CONTINUITY OF EIGENFUNCTIONS OF UNIQUELY ERGODIC DYNAMICAL SYSTEMS AND INTENSITY OF BRAGG PEAKS

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ABSTRACT. We study uniquely ergodic dynamical systems over locally compact, sigma-compact Abelian groups. We characterize uniform convergence in Wiener/Wintner type ergodic theorems in terms of continuity of the limit. Our results generalize and unify earlier results of Robinson and Assani respectively.

We then turn to diffraction of quasicrystals and show how the Bragg peaks can be calculated via a Wiener/Wintner type result. Combining these results we prove a version of what is sometimes known as Bombieri/Taylor conjecture.

Finally, we discuss various examples including deformed model sets, percolation models, random displacement models, and linearly repetitive systems.

1. INTRODUCTION

This paper is devoted to two related questions. One question concerns (uniform) convergence in the Wiener/Winter ergodic theorem. The other question deals with calculating the intensities of Bragg peaks in the diffraction of quasicrystals and, in particular, with the so called Bombieri/Taylor conjecture. As shown below the calculation of Bragg peaks can be reduced to convergence questions in certain ergodic theorems. The ergodic theorems of the first part then allow us to prove a version of the Bombieri/Taylor conjecture. Let us give an outline of these topics in this section. More precise statements and definitions will be given in the subsequent sections.

Consider a topological dynamical system (Ω, α) over a locally compact, σ-compact Abelian group G. Let ξ belong to the dual group of G and let (B_n) be a van Hove sequence. We study convergence of averages of the form

$$(*) \qquad \frac{1}{|B_n|}\int_{B_n} \overline{(\xi, s)} f(\alpha_{-s}\omega) ds.$$

Due to the von Neumann ergodic theorem and the Birkhoff ergodic theorem, it is known that these averages converge in L^2 and pointwise to the projection $E_T(\{\xi\})f$ of f on the eigenspace of ξ. In fact (for $G = \mathbb{R}$ or $G = \mathbb{Z}$) the set of $\omega \in \Omega$, where pointwise convergence fails, can be chosen uniformly in ξ. This is known as Wiener/Wintner ergodic theorem after [70].

Now, consider a uniquely ergodic (Ω, α). Unique ergodicity of (Ω, α) is equivalent to uniform (in $\omega \in \Omega$) convergence in $(*)$ for $\xi \equiv 1$ and continuous f. Thus, in this case one might expect uniform convergence for arbitrary ξ and continuous f on Ω. The first result of this paper, Theorem 1 in Section 3, characterizes validity of uniform convergence. It is shown to hold whenever possible, viz if and only if the limit $E_T(\{\xi\})f$ is continuous.

This generalizes earlier results of Robinson [57] for $G = \mathbb{R}^d$ and $G = \mathbb{Z}^d$. More precisely, Robinson's results state uniform convergence in two situations, viz for continuous eigenvalues ξ and for ξ outside the set of eigenvalues. To us the main achievement of our result is not so much the generalization of Robinson's results but rather our new proof. It does not require

any case distinctions but only continuity of the limit. Our line of argument is related to work of Furman on uniform convergence in subadditive ergodic theorems [19].

We then study dependence of convergence on ξ. Here, again, our result, Theorem 2 in Section 4, gives a uniformity statement, provided the limit has strong enough continuity properties in ξ. This result generalizes a result of Assani [2], where the limit is identically zero (and thus has the desired continuity properties). In fact, Theorem 2 unifies the results of Assani and Robinson.

While these results are of independent interest, here they serve as tool in the study of aperiodic order. This is discussed next.

Aperiodic order is a specific form of (dis)order intermediate between periodicity and randomness. It has attracted a lot of attention both in physics and in mathematics in recent years, see e.g. the monographs and conference proceedings [6, 29, 45, 51, 59]. This is due to its intriguing properties following from its characteristic intermediate form of (dis)order. In particular, the interest rose substantially after the actual discovery of physical substances, later called quasicrystals, which exhibit such a form of (dis)order [60, 28].

These solids were discovered in diffraction experiments by their unusual diffraction patterns. These patterns have, on the one hand, many points, called Bragg peaks, indicating long range order. On the other hand these patterns have symmetries incompatible with a lattice structure. Hence, these systems are not periodic. Put together, these solids exhibit long range aperiodic order. Investigation of mathematical diffraction theory is a key point in the emerging theory of aperiodic order, see the survey articles [7, 25, 33, 36, 48] and references given there.

The main object of diffraction theory is the diffraction measure $\widehat{\gamma}$ associated to the structure under investigation (see e.g. the book [14]). This measure describes the outcome of a physical diffraction experiment. The sharp spots appearing in a diffraction experiment known as Bragg peaks are then given as the point part of $\widehat{\gamma}$ and the intensity of a Bragg peak ξ is given by $\widehat{\gamma}(\{\xi\})$. According to these considerations central problems in mathematical diffraction theory are to

- prove pure pointedness of $\widehat{\gamma}$ or at least existence of a "large" point component of $\widehat{\gamma}$ for a given structure,
- explicitly determine ξ with $\widehat{\gamma}(\{\xi\}) > 0$ and calculate $\widehat{\gamma}(\{\xi\})$ for them.

Starting with the work of Hof [23], these two problems have been studied intensely over the last two decades for various models (see references above). The two main classes of models are primitive substitutions and cut and project models. Prominent examples such as the Fibonacci model or Penrose tilings belong to both classes [59].

From the very beginning the use of dynamical systems has been a most helpful tool in these investigations. The basic idea is to not consider one single structure but rather to assemble all structures with the "same" form of (dis)order (see e.g. [54]). This assembly will be invariant under translation and thus give rise to a dynamical system.

There is then a result of Dworkin [17] showing that the diffraction spectrum is contained in the dynamical spectrum (see as well the results of van Enter/Miękisz [18] for closely related complementary results). This so called Dworkin argument has been extended and applied in various contexts. In particular it has been the main tool in proving pure point diffraction by deducing it from pure point dynamical spectrum [58, 25, 64, 62]. Recently it has even been shown that pure point dynamical spectrum is equivalent to pure point diffraction [40, 3, 22] and that the set of eigenvalues is just the group generated by the Bragg peaks [3].

These results can be understood as (at least) partially solving the first problem mentioned above by relating the set of Bragg peaks to the eigenvalues of the associated dynamical system.

As for the second problem, the main line of reasoning goes as follows: Let the structure under investigation be given by a uniformly discrete relatively dense point set $\varLambda$ in $\mathbb{R}^d$. For $B \subset \mathbb{R}^d$ bounded with non-empty interior and $\xi \in \mathbb{R}^d$ define $c_B^\xi(\varLambda) := \frac{1}{|B|}\sum_{x\in\varLambda\cap B}\exp(-2\pi i\xi x)$, where $|\cdot|$ denotes Lebesgue measure. Then, the following should hold

$$(**) \qquad \widehat{\gamma}(\{\xi\}) = \lim_{n\to\infty} |c_{C_n}^\xi(\varLambda)|^2,$$

where C_n denotes the cube around the origin with side length $2n$. In fact, this is a crucial equality both in numerical simulations and in theoretical considerations. It is sometimes discussed under the heading of "Bombieri/Taylor conjecture". In their work [10, 11] Bombieri/Taylor state (for special one-dimensional systems) that the Bragg peaks are given by those ξ for which $\lim_{n\to\infty} c_{C_n}^\xi(\varLambda) \neq 0$. They do not give a justification for their statement and it then became known as their conjecture [23, 25].

Since then various works have been devoted to proving existence of $\lim_{n\to\infty} c_{C_n}^\xi(\varLambda)$ and rigorously justifying the validity of $(**)$. While the case of general uniquely ergodic systems is open, it has been shown by Hof in [23] that $(**)$ follows whenever a rather uniform convergence of $c_{B_n}^\xi(\varLambda)$ for van Hove sequences (B_n) is known (see the work [1] for a complementary result). This, in turn has been used to obtain validity of $(**)$ for model sets [25] and for primitive substitutions [20] (see Theorem 5.1 in [64] for related material as well).

Also, it has been mentioned in various degrees of explicitness [23, 25, 63, 33] that this uniform convergence of $c_{B_n}^\xi(\varLambda)$ follows from or is related to continuity of eigenfunctions due to Robinson's results [57] once one is in a dynamical system setting. So far no proofs for these statements seem to have appeared.

These questions are addressed in the second part of the paper. Our results show that $\widehat{\gamma}(\{\xi\})$ is related to a specific eigenfunction. More precisely, we proceed as follows.

In Section 5 we first discuss some background on diffraction and then introduce the measure dynamical setting from Baake/Lenz [3]. This setting has the virtue of embracing the two most common frameworks for the mathematical modeling of quasicrystals viz the framework of point sets used in mathematical diffraction theory starting with the work [23] and the framework of bounded functions brought forward in [8]. They are are both just special cases of the measure approach. Using some material from [3] we derive Theorem 3 in Section 5. It shows that $\widehat{\gamma}(\{\xi\})$ is the norm square of a certain specific eigenfunction to ξ. This does not require any ergodicity assumptions and relies solely on the Stone/von Neumann spectral theorem for unitary representations and [3].

Depending on whether one has the von Neumann ergodic theorem, or the Birkhoff ergodic theorem or a uniform Wiener-Wintner type theorem at one's disposal, one can then calculate $\widehat{\gamma}(\{\xi\})$ as L^2-limit, almost-sure limit or uniform limit of averages of the form $(*)$. These averages can then be related to the Fourier type averages in $(**)$ by Lemma 8 to give the corresponding L^2, almost-sure pointwise and uniform convergence statement in $(**)$. This is summarized in Theorem 5 in Section 6. In particular, (b) of Theorem 5 shows that an almost sure justification of Bombieri/Taylor holds in arbitrary ergodic dynamical systems and does not require any continuity assumptions on the eigenfunction to ξ. As a consequence we obtain in Corollary 3 a variant of the Bombieri/Taylor conjecture valid for arbitrary uniquely ergodic systems.

These abstract results can be used to reprove validity of $(**)$ for the two most common models of aperiodic order viz primitive substitution models and models arising from cut and project schemes (see first remark in Section 6). More importantly, they can be used to prove validity of $(**)$ for a variety of new models. In particular, they allow one to obtain variants of the Bombieri/Taylor conjecture for several models arising from strictly aperiodically ordered ones by some randomization or smearing out process.

In fact, based on the results of this paper a strong version of the Bombieri/Taylor conjecture is proven by Lenz/Strungaru [38] for the class of deformed model sets earlier studied in [9, 4, 22] and by Lenz/Richard [37] for dense Dirac combs introduced in [56]. These results are shortly sketched in Section 7.

Moreover, as shown in Section 8 our abstract results yield almost sure validity of the Bombieri/Taylor conjecture for both percolation models and random displacement models based on aperiodic order. These models are more realistic in that they take into account defects and thermal motion in solids respectively. Percolation models based on aperiodic order were introduced by Hof [26]. There, equality of various critical probabilities is shown. An extension of Hof's work to graphs together with an application to random operators is then given in recent work of Müller/Richard [50]. Random displacement in diffraction for a single object (rather than a dynamical system) is discussed by Hof in [24]. In fact, convergence of diffraction for both percolation and random displacement models (and quite some further models) has recently been studied by Külske [30, 31]. His results give rather universal convergence of approximants. However, they deal with a smoothed version of diffraction. Thus, they do not seem to give validity of the Bombieri/Taylor conjecture. In this sense, our results complement the corresponding results of [30]. We refer to Section 8 for further details.

In the final section, we study so called linearly repetitive Delone dynamical systems, introduced by Lagarias/Pleasants in [34], and their subshift counterparts, so called linearly recurrent subshifts, studied e.g. by Durand in [16]. These examples have attracted particular attention in recent years and have been brought forward as models for perfectly ordered quasicrystals in [34]. Quite remarkably, continuity of eigenfunctions fails for these models in general as recently shown in [12]. Nevertheless, we are able to establish validity of $(**)$ for these models. More generally, we show that uniform convergence of the modules of the expressions in $(*)$ holds (while uniform convergence of the expressions themselves may fail) and this gives validity of $(**)$ as discussed above. This is based on the subadditive ergodic theorems from [15, 35]. Let us emphasize that convergence in these cases does not hold uniformly in the van Hove sequences but only for so-called Fisher sequences.

2. Dynamical systems

Our general framework deals with actions of locally compact Abelian groups on compact spaces. Thus, we start with some basic notation and facts concerning these topics. These will be used throughout the paper.

Whenever X is a σ-compact locally compact space (by which we include the Hausdorff property), the space of continuous functions on X is denoted by $C(X)$ and the subspace of continuous functions with compact support by $C_c(X)$. For a bounded function f on X, we define the supremum norm by

$$\|f\|_\infty := \sup\{|f(x)| : x \in X\}.$$

Equipped with this norm, the space $C_K(X)$ of complex continuous functions on X with support in the compact set $K \subset G$ becomes a complete normed space. Then, the space

$C_c(G)$ is equipped with the locally convex limit topology induced by the canonical embedding $C_K(X) \hookrightarrow C_c(X)$, $K \subset G$, compact.

As X is a topological space, it carries a natural σ-algebra, namely the Borel σ-algebra generated by all closed subsets of X. The set $\mathcal{M}(X)$ of all complex regular Borel measures on G can then be identified with the space $C_c(X)^*$ of complex valued, continuous linear functionals on $C_c(G)$. This is justified by the Riesz-Markov representation theorem, compare [52, Ch. 6.5] for details. The space $\mathcal{M}(X)$ carries the vague topology, i.e., the weakest topology that makes all functionals $\mu \mapsto \int_X f \, \mathrm{d}\mu$, $\varphi \in C_c(X)$, continuous. The total variation of a measure $\mu \in \mathcal{M}(X)$ is denoted by $|\mu|$.

Now fix a σ-compact locally compact Abelian (LCA) group G. Denote the Haar measure on G by θ_G. The dual group of G is denoted by $\widehat{G}$, and the pairing between a character $\xi \in \widehat{G}$ and $t \in G$ is written as (ξ, t). Whenever G acts on the compact space Ω by a continuous action

$$\alpha\colon\ G \times \Omega \ \longrightarrow\ \Omega\,, \quad (t,\omega) \ \mapsto\ \alpha_t(\omega)\,,$$

where $G \times \Omega$ carries the product topology, the pair (Ω, α) is called a *topological dynamical system* over G. We will often write $\alpha_t\omega$ for $\alpha_t(\omega)$. An α-invariant probability measure is called *ergodic* if every measurable invariant subset of Ω has measure zero or measure one. The dynamical system (Ω, α) is called *uniquely ergodic* if there exists a unique α-invariant probability measure.

We will need two further pieces of notation. A map Φ between dynamical system (Ω, α) and (Ω', α') over G is called a *G - map* if $\Phi(\alpha_t(\omega)) = \alpha'_t(\Phi(\omega))$ for all $\omega \in \Omega$ and $t \in G$. A continuous surjective G - map is called a *factor map.*

Given an α-invariant probability measure m, we can form the Hilbert space $L^2(\Omega, m)$ of square integrable measurable functions on Ω. This space is equipped with the inner product

$$\langle f, g\rangle \ =\ \langle f, g\rangle_\Omega \ :=\ \int_\Omega \overline{f(\omega)}\, g(\omega)\, \mathrm{d}m(\omega).$$

The action α gives rise to a unitary representation $T = T^{(\Omega,\alpha,m)}$ of G on $L^2(\Omega, m)$ by

$$T_t\colon\ L^2(\Omega, m) \ \longrightarrow\ L^2(\Omega, m)\,, \quad (T_t f)(\omega) \ :=\ f(\alpha_{-t}\omega)\,,$$

for every $f \in L^2(\Omega, m)$ and arbitrary $t \in G$. An $f \in L^2(\Omega, m)$ is called an *eigenfunction* of T with *eigenvalue* $\xi \in \widehat{G}$ if $T_t f = (\xi, t) f$ for every $t \in G$. An eigenfunction (to ξ, say) is called *continuous* if it has a continuous representative f with

$$f(\alpha_{-t}\omega) = (\xi, t) f(\omega), \text{ for all } \omega \in \Omega \text{ and } t \in G.$$

By Stone's theorem, compare [42, Sec. 36D], there exists a projection valued measure

$$E_T\colon \text{ Borel sets of } \widehat{G} \ \longrightarrow\ \text{projections on } L^2(\Omega, m)$$

with

$$\langle f, T_t f\rangle \ =\ \int_{\widehat{G}} (\xi, t)\, \mathrm{d}\langle f, E_T(\xi) f\rangle \ :=\ \int_{\widehat{G}} (\xi, t)\, \mathrm{d}\rho_f(\xi)\,, \tag{1}$$

where ρ_f is the measure on $\widehat{G}$ defined by $\rho_f(B) := \langle f, E_T(B) f\rangle$.

We will be concerned with averaging procedures along certain sequences. To do so we define for $Q, P \subset G$ the P boundary $\partial^P Q$ of Q by

$$\partial^P Q := ((P + Q) \setminus Q^\circ) \cup ((-P + \overline{G \setminus Q}) \cap Q)),$$

where the bar denotes the closure of a set and the circle denotes the interior. As G is σ-compact, there exists a sequence $\{B_n : n \in \mathbb{N}\}$ of open, relatively compact sets $B_n \subset G$ with $\overline{B_n} \subset B_{n+1}$, $G = \bigcup_{n\geq 1} B_n$, and

$$\lim_{n\to\infty} \frac{\theta_G(\partial^K B_n)}{\theta(B_n)} = 0,$$

for every compact $K \subset G$ see [62] for details. Such a sequence is called a *van Hove sequence*.

The relevant averaging operator is defined next.

Definition 1. *Let (Ω, α) be a dynamical system over G. For $\xi \in \widehat{G}$, $B \subset G$ relatively compact with non-empty interior and a bounded measurable f on Ω, the bounded measurable function $A_B^\xi(f)$ on Ω is defined by*

$$A_B^\xi(f)(\omega) := \frac{1}{\theta_G(B)} \int_B \overline{(\xi, s)} f(\alpha_{-s}\omega) ds.$$

In particular, A_B^ξ maps $C(\Omega)$ into itself.

In this context the von Neumann ergodic theorem (see e.g. [32, Thm. 6.4.1]) gives the following.

Lemma 1. *Let (Ω, α) be a dynamical system over G with α-invariant probability measure m and associated spectral family E_T. Then,*

$$A_{B_n}^\xi(f) \longrightarrow E_T(\{\xi\})f,\ n \to \infty,$$

in $L^2(\Omega, m)$ for any $f \in C(\Omega)$ and every van Hove sequence (B_n).

There is also a corresponding well-known pointwise statement.

Lemma 2. *Let (Ω, α) be a dynamical system and m an ergodic invariant probability measure on Ω. Let (B_n) be a van Hove sequence in G along which the Birkhoff ergodic theorem holds. Then, $A_{B_n}^\xi(f)$ converges almost surely (and in $L^2(\Omega, m)$) to $E_T(\{\xi\})f$ for every $f \in C(\Omega)$.*

Remark. As shown by Lindenstrauss in [39], every amenable group admits a van Hove sequence along which the Birkhoff ergodic theorem holds.

Proof of Lemma 2. Let $\mathbb{T}$ be the unit circle and consider the dynamical system $\Omega \times \mathbb{T}$ with action of G given by $\alpha_s(\omega, \theta)) = (\alpha_s\omega, (\xi, s)\theta)$. Then, the statement follows from Birkhoff ergodic theorem applied to $F(\omega, \theta) = \theta f(\omega)$. $\square$

In order to prove our abstract results, we need two more preparatory results.

Lemma 3. *Let (Ω, α) be a dynamical system over G. Let Q, P be open, relatively compact non-empty subsets of G. Then,*

$$\|A_Q^\xi(f) - A_P^\xi(A_Q^\xi(f))\|_\infty \leq \frac{\theta_G(\partial^{P\cup(-P)}Q)}{\theta_G(Q)} \|f\|_\infty$$

for every $f \in C(\Omega)$.

Proof. For $t \in G$ a direct calculation shows

$$\begin{aligned} |A_Q^\xi(f)(\omega) - \overline{(\xi, t)} A_Q^\xi(\alpha_{-t}\omega)| &= \frac{1}{\theta_G(Q)} \left| \int_Q f(\alpha_{-s}\omega)\overline{(\xi, s)} ds - \int_{t+Q} f(\alpha_{-s}\omega)\overline{(\xi, s)} ds \right| \\ &\leq \frac{\theta_G(Q \setminus (t+Q) \cup (t+Q) \setminus Q)}{\theta_G(Q)} \|f\|_\infty. \end{aligned}$$

For $t \in P$, we have $Q \setminus (t+Q) \cup (t+Q) \setminus Q \subset \partial^{P\cup(-P)} Q$ and the lemma follows. $\square$

The following lemma is certainly well known. We include a proof for completeness.

Lemma 4. *Let (Ω, α) be uniquely ergodic with unique α-invariant probability measure m. Let $K \subset \Omega$ be compact and denote the characteristic function of K by χ_K. Then, for every van Hove sequence (B_n)*

$$\limsup_{n\to\infty} \frac{1}{|B_n|} \int_{B_n} \chi_K(\alpha_{-s}\omega) ds \leq m(K)$$

uniformly in $\omega \in \Omega$.

Proof. As Ω is compact, the measure m is regular. In particular, for every $\varepsilon > 0$, we can find an open set V containing K with $m(V) \leq m(K) + \varepsilon$. By Urysohns lemma, we can then find a continuous function $h : \Omega \longrightarrow [0,1]$ with support contained in V and $h \equiv 1$ on K. By construction, $\int_\Omega h(\omega) dm(\omega) \leq m(K) + \varepsilon$ and

$$0 \leq \frac{1}{|B_n|} \int_{B_n} \chi_K(\alpha_{-s}\omega) ds \leq \frac{1}{|B_n|} \int_{B_n} h(\alpha_{-s}\omega) ds$$

for every $\omega \in \Omega$. By unique ergodicity, $\frac{1}{|B_n|} \int_{B_n} h(\alpha_{-s}\omega) ds$ converges uniformly on Ω to $\int_\Omega h(\omega) dm(\omega)$. Putting this together, we obtain

$$\limsup_{n\to\infty} \frac{1}{|B_n|} \int_{B_n} \chi_K(\alpha_{-s}\omega) ds \leq \int_\Omega h(\omega) dm(\omega) \leq m(K) + \varepsilon$$

uniformly on Ω. As $\varepsilon > 0$ is arbitrary, the statement of the lemma follows. $\square$

3. Uniform Wiener-Wintner type results

In this section we discuss the following theorem.

Theorem 1. *Let (Ω, α) be a uniquely ergodic dynamical system over G with α-invariant probability measure m. Let $\xi \in \widehat{G}$ and $f \in C(\Omega)$ be arbitrary. Then, the following assertions are equivalent:*

(i) *The function $E_T(\{\xi\})f$ has a continuous representative g satisfying $g(\alpha_{-s}\omega) = (\xi, s)\, g(\omega)$ for every $s \in G$ and $\omega \in \Omega$.*

(ii) *For some (and then every) van Hove sequence (B_n), the averages $A^\xi_{B_n}(f)$ converge uniformly, that is to say w.r.t. the supremum norm to a function g.*

Remark. (a) The hard part of the theorem is the implication $(i) \Longrightarrow (ii)$. Note that (i) comprises three situations:

- ξ is an eigenvalue of T with a continuous eigenfunction.
- ξ is not an eigenvalue at all (then $g \equiv 0$).
- ξ is an eigenvalue and f is perpendicular to the corresponding eigenfunctions (then, again, $g \equiv 0$).

(b) Our proof relies on the von Neumann ergodic theorem, Lemma 1, and unique ergodicity only. Thus, the proof carries immediately over to give a semigroup version e.g. for actions of $\mathbb{N}$, as the von Neumann ergodic theorem is known then.

(c) The statement $(i) \Longrightarrow (ii)$ is given for the first two situations of (a) separately by Robinson in [57] for actions of $G = \mathbb{Z}^d$ and $G = \mathbb{R}^d$. Actually, his proof also works for the third situation. Our proof is different in this case and works for all three situations at the

same time. Robinson also has a version for actions of $\mathbb{N}$. As mentioned in (b), this can be shown by our method as well.

Proof of Theorem 1:

(ii)$\Longrightarrow$ (i): By assumption there exists a van Hove sequence (B_n) such that the averages $(A_{B_n}^{\xi}(f))$ converge uniformly to a function g. As each $A_{B_n}^{\xi}(f)$ is continuous, so is g. Moreover, a direct calculation shows

$$g(\alpha_{-t}\omega) = \lim_{n\to\infty} A_{B_n}^{\xi}(f)(\alpha_{-t}\omega) = \lim_{n\to\infty}(\xi,t)A_{t+B_n}^{\xi}(f)(\omega) = (\xi,t)g(\omega)$$

for all $t \in G$ and $\omega \in \Omega$. By Lemma 1, $A_{B_n}^{\xi}(f)$ converges in $L^2(\Omega,m)$ to $E_T(\{\xi\})f$. Thus, the uniform convergence of the $A_{B_n}^{\xi}(f)$ to g implies $g = E_T(\{\xi\})f$. This finishes the proof of this implication. (The fact that convergence holds for every van Hove sequence will be proven along the way of (i) $\Longrightarrow$ (ii).)

(i)$\Longrightarrow$ (ii): Let (B_n) be an arbitrary van Hove sequence.

Let $\varepsilon > 0$ be given. We show that

$$(\sharp) \qquad \|A_{B_n}^{\xi}(f) - g\|_\infty \leq 3(1 + \|f\|_\infty + \|g\|_\infty)\varepsilon$$

for all sufficiently large n.

By assumption (i) and Lemma 1, $A_{B_n}^{\xi}(f)$ converges in $L^2(\Omega,m)$ to the continuous function g. This implies $\lim_{n\to\infty}\mu(\Omega_n) = 1$ where

$$\Omega_n := \{\omega \in \Omega : |A_{B_n}^{\xi}(f)(\omega) - g(\omega)| < \varepsilon\}.$$

In particular, for sufficiently large N, we have

$$m(\Omega_N) \geq 1 - \varepsilon.$$

Fix such an N and set $b := A_{B_N}^{\xi}(f)$.

As both b and g are continuous, the set Ω_N is open. Thus, its complement $K := \Omega \setminus \Omega_N$ is compact. Let χ_{Ω_N} and χ_K be the characteristic functions of Ω_N and K respectively. Thus, in particular,

- $\chi_{\Omega_N}(\omega) > 0$ implies $\omega \in \Omega_N$, i.e. $|b(\omega) - g(\omega)| < \varepsilon$.
- $m(K) \leq \varepsilon$ (as $m(\Omega_N) \geq 1 - \varepsilon$).

Note that $A_{B_n}^{\xi}(b) = A_{B_N}^{\xi}(A_{B_n}^{\xi}(f))$ by Fubini's theorem and $A_{B_n}^{\xi}(g) = g$ by the invariance assumption on g. Thus, we can estimate

$$\begin{aligned}
\|A_{B_n}^{\xi}(f) - g\|_\infty &\leq \|A_{B_n}^{\xi}(f) - A_{B_N}^{\xi}(A_{B_n}^{\xi}(f))\|_\infty + \|A_{B_n}^{\xi}(b) - A_{B_n}^{\xi}(g)\|_\infty \\
&\leq \|A_{B_n}^{\xi}(f) - A_{B_N}^{\xi}(A_{B_n}^{\xi}(f))\|_\infty + \|A_{B_n}^{\xi}(\chi_{\Omega_N}(b-g))\|_\infty \\
&+ \|A_{B_n}^{\xi}(\chi_K\, b)\|_\infty + \|A_{B_n}^{\xi}(\chi_K\, g)\|_\infty.
\end{aligned}$$

We estimate the last four terms:

Term 1: By Lemma 3, this term can be estimated from above by

$$\frac{\theta_G(\partial^{B_N\cup(-B_N)}B_n)}{\theta_G(B_n)}\|f\|_\infty.$$

As (B_n) is a van Hove sequence, this term is smaller than ε for sufficiently large n.

Term 2: As $\chi_{\Omega_N}(\omega) > 0$ implies $|b(\omega) - g(\omega)| < \varepsilon$, the estimate $\|\chi_{\Omega_N}(b-g)\|_\infty < \varepsilon$ holds. This gives $\|A^\xi_{B_n}(\chi_{\Omega_N}(b-g))\|_\infty \leq \|\chi_{\Omega_N}(b-g)\|_\infty < \varepsilon$ and the second term is smaller than ε for every $n \in \mathbb{N}$.

Term 3: A short calculation shows

$$\|A^\xi_{B_n}(\chi_K\, b)\|_\infty \leq \frac{1}{\theta_G(B_n)} \int_{B_n} \chi_K(\alpha_{-s}\omega) ds \|b\|_\infty.$$

As K is compact with $m(K) \leq \varepsilon$, we can then infer from Lemma 4 that $\frac{1}{\theta_G(B_n)} \int_{B_n} \chi_K(\alpha_{-s}\omega) ds$ is uniformly bounded by 2ε for large enough n. As $\|b\|_\infty \leq \|f\|_\infty$ by definition of b, we conclude that the third term is smaller than $2\varepsilon\|f\|_\infty$ for sufficiently large n.

Term 4: Using the same arguments as in the treatment of the third term, we see that the fourth term can be estimated above by $2\varepsilon\|g\|_\infty$ for sufficiently large n.

Putting the estimates together we infer ($\sharp$). $\square$

We can use the above method of proof to give a proof for the key technical lemma of [57] in our context.

Lemma 5. *Let (Ω, α) be uniquely ergodic. Let $f \in C(\Omega)$ and $\xi \in \widehat{G}$ be arbitrary. Then,* $\lim_{n\to\infty} \|A^\xi_{B_n}\|_\infty = \sqrt{\langle E_T(\{\xi\})f, E_T(\{\xi\})f\rangle}$.

Proof. For each $\varepsilon > 0$ and $N \in \mathbb{N}$, Lemma 3 gives

$$\|A^\xi_{B_n}(f)\|_\infty \leq \|A^\xi_{B_N}(A^\xi_{B_n}(f))\|_\infty + \varepsilon \leq \|A^\xi_{B_N}(f)\|_\infty + \varepsilon$$

for sufficiently large $n \in \mathbb{N}$. This easily shows existence of the limit $\lim_{n\to\infty} \|A^\xi_{B_n}(f)\|_\infty$.

Now, by the von Neumann ergodic theorem, we have L^2-convergence of $A^\xi_{B_n}(f)$ to $E_T(\{\xi\})f$. This gives L^2-convergence of $|A^\xi_{B_n}(f)|$ to $|E_T(\{\xi\})f|$ and the latter is almost surely equal to $c := \sqrt{\langle E_T(\{\xi\})f, E_T(\{\xi\})f\rangle}$. As each L^2 converging sequence contains an almost surely converging subsequence, we infer that $\lim_{n\to\infty} \|A^\xi_{B_n}(f)\|_\infty \geq c$.

It remains to show $\lim_{n\to\infty} \|A^\xi_{B_n}(f)\|_\infty \leq c$. Here, we mimic the previous proof: Choose $\varepsilon > 0$ arbitrary. By L^2-convergence of $|A^\xi_{B_n}(f)|$ to the constant function c, we can find an $N \in \mathbb{N}$ such that $m(\Omega_N) \geq 1 - \varepsilon$, where

$$\Omega_N := \{\omega \in \Omega : ||A^\xi_{B_N}(f)(\omega)| - c| < \varepsilon\}.$$

Note that Ω_N is open and hence $\Omega \setminus \Omega_N$ is compact. For n large enough we then have (see above)

$$\|A^\xi_{B_n}(f)\|_\infty \leq \|A^\xi_{B_N}(f)\|_\infty + \varepsilon \leq \|A^\xi_{B_n}(\chi_{\Omega_N} A^\xi_{B_N}(f))\|_\infty + \|A^\xi_{B_n}(\chi_{\Omega\setminus\Omega_N} A^\xi_{B_N}(f))\|_\infty + \varepsilon.$$

For $\omega \in \Omega_N$, we have $|A^\xi_{B_N}(f)(\omega)| \leq c + \varepsilon$. Hence, the first term on the right hand side can be estimated by $c + \varepsilon$. The second term on the right hand side can be estimated by $\|f\|_\infty \frac{1}{|B_n|} \int_{B_n} \chi_{\Omega\setminus\Omega_N}(\alpha_s\omega) ds$. By Lemma 4, $\frac{1}{|B_n|} \int_{B_n} \chi_{\Omega\setminus\Omega_N}(\alpha_s\omega) ds$ is smaller than $2\varepsilon = m(\Omega \setminus \Omega_N) + \varepsilon$ for sufficiently large n. This finishes the proof of the lemma. $\square$

4. Unifying Theorem 1 and a result of Assani

In this section we present the following consequence and in fact generalization of the hard part of Theorem 1, which generalizes a result of Assani as well.

Theorem 2. *Let (Ω, α) be a uniquely ergodic dynamical system over G with α-invariant probability measure m. Let $f \in C(\Omega)$ and $K \subset \widehat{G}$ be given such that, firstly, for every $\xi \in K$ the function $E_T(\{\xi\})f$ is continuous with $E_T(\{\xi\})f(\alpha_{-s}\omega) = (\xi, s)E_T(\{\xi\})f$ for all $\omega \in \Omega$ and $s \in G$ and, secondly, $K \longrightarrow C(\Omega)$, $\xi \mapsto E_T(\{\xi\})f$, is continuous. Then,*

$$\lim_{n\to\infty} \sup_{\xi\in K} \|A^{\xi}_{B_n}(f) - E_T(\{\xi\})f\|_\infty = 0$$

for every van Hove sequence (B_n).

Remark. (a) Certainly the theorem contains the case $K = \{\xi\}$ and we recover the implication $(i) \Longrightarrow (ii)$ of Theorem 1.

(b) The proof of the theorem relies on the previous theorem and compactness. Thus, again, there is a semigroup version e.g. for actions of $\mathbb{N}$.

The theorem has the following immediate corollary.

Corollary 1. *Let G be discrete and let (Ω, α) be a uniquely ergodic dynamical system over G with α-invariant probability measure m. Let $f \in C(\Omega)$ be given such that $E_T(\{\xi\})f = 0$ for every $\xi \in \widehat{G}$. Then,*

$$\lim_{n\to\infty} \sup_{\xi\in \widehat{G}} \|A^{\xi}_{B_n}(f)\|_\infty = 0$$

for every van Hove sequence (B_n).

Remark. For $G = \mathbb{Z}$ the corollary was proven by Assani 1993 in an unpublished manuscript. A published proof can be found in his book [2]. In fact, the book gives the semigroup version for actions of $\mathbb{N}$.

Proof of Theorem 2: Define for each $n \in \mathbb{N}$ the function $b_n : K \longrightarrow \mathbb{R}$, $\xi \mapsto \|A^{\xi}_{B_n}(f) - E_T(\{\xi\})f\|_\infty$. Then, each b_n is continuous by our assumptions and

$$b_n(\xi) \longrightarrow 0,\ n \to \infty, \tag{2}$$

for each $\xi \in K$ by Theorem 1. Moreover, by the invariance assumption on $E_T(\{\xi\})f$, we have $A^{\xi}_{B_n}(E_T(\{\xi\})f) = E_T(\{\xi\})f$ for all $n \in \mathbb{N}$. Thus, Lemma 3 and direct arguments give for all $n, N \in \mathbb{N}$:

$$\begin{aligned}
b_n(\xi) &= \|A^{\xi}_{B_n}(f) - E_T(\{\xi\})f\|_\infty = \|A^{\xi}_{B_n}(f) - A^{\xi}_{B_n}(E_T(\{\xi\})f)\|_\infty \\
&\le \|A^{\xi}_{B_n}(f) - A^{\xi}_{B_N}(A^{\xi}_{B_n}(f))\|_\infty + \|A^{\xi}_{B_n}(A^{\xi}_{B_N}(f)) - A^{\xi}_{B_n}(E_T(\{\xi\})f)\|_\infty \\
&\le \frac{\theta_G(\partial^{B_N\cup(-B_N)} B_n)}{\theta_G(B_n)} \|f\|_\infty + \|A^{\xi}_{B_N}(f) - E_T(\{\xi\})f\|_\infty \\
&= \frac{\theta_G(\partial^{B_N\cup(-B_N)} B_n)}{\theta_G(B_n)} \|f\|_\infty + b_N(\xi).
\end{aligned}$$

As (B_n) is a van Hove sequence this easily shows that the sequence (b_n) has the following monotonicity property: For each $N \in \mathbb{N}$ and $\varepsilon > 0$, there exists an $n_0(N, \varepsilon) \in \mathbb{N}$ with

$$b_n(\xi) \leq b_N(\xi) + \varepsilon \tag{3}$$

for all $n \geq n_0(N, \varepsilon)$ and all $\xi \in K$. Given (2) and (3), the theorem follows from compactness of K and continuity of the b_n, $n \in \mathbb{N}$, by standard reasoning. □

5. Diffraction theory

In this section we present a basic setup for diffraction (see e.g. [14]). For models with aperiodic order this framework has been advocated by Hof [23] and become a standard by now (see introduction for references). The crucial quantity is a measure, called the diffraction measure and denoted by $\widehat{\gamma}$. It models the outcome of a diffraction experiment by representing the intensity (per unit volume). We begin the section with a short discussion of background material. We then discuss the measure based approach developed recently [3, 4]. We also present a consequence of [3] viz Theorem 3 (and its corollary), which will be used in the next section. It may be of independent interest. We then finish this section by elaborating on how the usual approach via point sets fits into the measure approach.

In a diffraction experiment a solid is put into an incoming beam of e.g. X rays. The atoms of the solid then interact with the beam and one obtains an out coming wave. The intensity of this wave is then measured on a screen. When modeling diffraction, the two basic principles are the following: Firstly, each point x in the solid gives rise to a wave $\xi \mapsto \exp(-ix\xi)$. The overall wave w is the sum of the single waves. Secondly, the quantity measured in an experiment is the intensity given as the square of the modulus of the wave function.

We start with by implementing this for a finite set $F \subset \mathbb{R}^d$. Each $x \in F$ gives rise to a wave $\xi \mapsto \exp(-ix\xi)$ and the overall wavefunction w_F induced by F is accordingly

$$w_F(\xi) = \sum_{x \in F} \exp(-ix\xi).$$

Thus, the intensity I_F is

$$I_F(\xi) = \sum_{x,y \in F} \exp(-i(x-y)\xi) = \widehat{(\sum_{x,y \in F} \delta_{x-y})}. \tag{4}$$

Here, δ_z is the unit point mass at z and $\widehat{\ }$ denotes the Fourier transform. When describing diffraction for a solid with many atoms it is common to model the solid by an infinite set in $\mathbb{R}^d$. When trying to establish a formalism as above for an infinite set $\varLambda$, one faces the problem that

$$w_\varLambda = \sum_{x \in \varLambda} \exp(-ix\xi)$$

diverges heavily and therefore does not make sense. This problem can not be overcome by interpreting the sum as a tempered distribution. The reason is that we are actually not interested in $w_\varLambda$ but rather in $|w_\varLambda|^2$. Now, neither modulus nor products are defined for distributions. There is a physical reason behind the divergence: The intensity of the whole set $\varLambda$ is really infinite. The correct quantity to consider is not the intensity but a normalized intensity viz the intensity per unit volume. It is given as

$$I = \lim_{n \to \infty} \frac{1}{|B_n|} I_{\varLambda \cap B_n}.$$

Of course, existence of this limit is not clear at all. In fact, we will even have to specify in which sense existence of the limit is meant. It turns out that existence of the limit in the vague sense is equivalent to existence of the limit

$$\gamma = \lim_{n\to\infty} \frac{1}{|B_n|} \sum_{x,y\in \Lambda\cap B_n} \delta_{x-y}$$

in the vague sense. In this case, I is the Fourier transform $\widehat{\gamma}$ of γ. Then, γ is known as autocorrelation function and $I = \widehat{\gamma}$ is known as diffraction measure. We are particularly interested in the point part of $\widehat{\gamma}$. The points $\xi \in \mathbb{R}^d$ with $\widehat{\gamma}(\{\xi\}) \neq 0$ are called *Bragg peaks*. The value $\widehat{\gamma}(\{\xi\})$ is called the *intensity of the Bragg peak*. Particularly relevant questions in this context are the following:

- When is $\widehat{\gamma}$ a pure point measure?
- Where are the Bragg peaks?
- What are the intensities of the Bragg peaks?

These questions have been discussed in a variety of settings by various people (see introduction). Here, we will now present the framework and (part of) the results concerning the first two questions developed in [3, 4]. The study of the last question is the main content of the remainder of the paper.

We will be concerned with suitable subsets of the set $\mathcal{M}(G)$ of measures on G. There is a canonical map

$$f : C_c(G) \longrightarrow C(\mathcal{M}(G)),\;\; f_\varphi(\mu) := \int_G \varphi(-s)\, d\mu(s). \tag{5}$$

The vague topology on $\mathcal{M}(G)$ is the smallest topology which makes all the f_φ, $\varphi \in C_c(G)$, continuous.

Let $C > 0$ and a relatively compact open set V in G be given. A measure $\mu \in \mathcal{M}(G)$ is called (C, V)*-translation bounded* if $|\mu|(t + V) \leq C$ for all $t \in G$. The set of all (C, V)-translation bounded measures is denoted by $\mathcal{M}_{C,V}(G)$. The set $\mathcal{M}_{C,V}(G)$ is a compact Hausdorff space in the vague topology. There is a canonical map

$$f : C_c(G) \longrightarrow C(\mathcal{M}_{C,V}(G)),\;\; f_\varphi(\mu) := \int_G \varphi(-s)\, d\mu(s).$$

Moreover, G acts on $\mathcal{M}_{C,V}(G)$ via a continuous action α given by

$$\alpha\colon\; G \times \mathcal{M}_{C,V}(G) \;\longrightarrow\; \mathcal{M}_{C,V}(G)\,, \quad (t,\mu) \;\mapsto\; \alpha_t\mu \quad \text{with} \quad (\alpha_t\mu)(\varphi) \;:=\; \int_G \varphi(s+t) d\mu(s).$$

Definition 2. (Ω, α) *is called a dynamical system on the translation bounded measures on* G (TMDS) *if there exist a constant* $C > 0$ *and a relatively compact open set* $V \subset G$ *such that* Ω *is a closed* α*-invariant subset of* $\mathcal{M}_{C,V}(G)$.

Having introduced our models, we can now discuss some key issues of diffraction theory. Let (Ω, α) be a TMDS, equipped with an α-invariant probability measure m.

Then, there exists a unique measure $\gamma = \gamma_m$ on G, called the *autocorrelation measure* (often called Patterson function in crystallography [14], though it is a measure in our setting) with

$$\gamma * \widetilde{\varphi} * \psi\,(t) = \langle f_\varphi, T_t f_\psi\rangle \tag{6}$$

for all $\varphi, \psi \in C_c(G)$ and $t \in G$. The convolution $\varphi * \psi$ is defined by $(\varphi * \psi)(t) = \int \varphi(t - s)\psi(s)\, \mathrm{d}s$. For $\psi \in C_c(G)$ the function $\widetilde{\psi} \in C_c(G)$ is defined by $\widetilde{\psi}(x) = \overline{\psi(-x)}$.

By (6) (applied with $t = 0$), the measure γ is positive definite. Therefore, its Fourier transform exists and is a positive measure $\widehat{\gamma}$. It is called the *diffraction measure*. As discussed in the beginning of this section, this measure describes the outcome of a diffraction experiment.

Taking Fourier transforms in (6) and (1) with $f = f_\varphi$, we obtain (see Proposition 7 in [3] for details)

$$\rho_{f_\varphi} = |\widehat{\varphi}|^2 \widehat{\gamma} \tag{7}$$

for every $\varphi \in C_c(G)$. This equation can be used to show that $\widehat{\gamma}$ is a pure point measure if and only if T has pure point spectrum [3], see [40, 62] as well. This equation also lies at the heart of the following theorem.

Theorem 3. *Let (Ω, α) be a TMDS with an α-invariant probability measure m and associated autocorrelation function γ. Let $\xi \in \widehat{G}$ be arbitrary. Then, there exists a unique $c_\xi \in L^2(\Omega, m)$ with*

$$E_T(\{\xi\}) f_\psi = \widehat{\psi}(\xi) c_\xi$$

for every $\psi \in C_c(G)$. The function c_ξ satisfies $\widehat{\gamma}(\{\xi\}) = \langle c_\xi, c_\xi \rangle$.

Proof. Uniqueness of such a c_ξ is clear. Existence and further properties can be shown as follows:

From (7) we obtain by a direct polarization argument that

$$(\#) \quad \langle f_\varphi, E_T(B) f_\psi \rangle = \int \chi_B \, \overline{\widehat{\varphi}} \, \widehat{\psi} \, d\gamma$$

for all $\varphi, \psi \in C_c(G)$ and $B \subset \widehat{G}$ measurable. Here, χ_B denotes the characteristic function of B. Note that $E_T(B)$ is a projection and therefore $\langle f_\varphi, E_T(B) f_\psi \rangle = \langle E_T(B) f_\varphi, E_T(B) f_\psi \rangle$ for arbitrary $\varphi, \psi \in C_c(G)$ and $B \subset \widehat{G}$ measurable.

Now, choose $\sigma \in C_c(G)$ with $\int_G \sigma(s) ds = 1$ and define $\sigma_\star \in C_c(G)$ by $\sigma_\star := (\xi, \cdot)\sigma$. Then, $\widehat{\sigma_\star}(\xi) = 1$. Define $c_\xi := E_T(\{\xi\}) f_{\sigma_\star}$. Then,

$$\langle c_\xi, c_\xi \rangle = \langle E_T(\{\xi\}) f_{\sigma_\star}, E_T(\{\xi\}) f_{\sigma_\star} \rangle = \langle f_{\sigma_\star}, E_T(\{\xi\}) f_{\sigma_\star} \rangle = \widehat{\gamma}(\{\xi\})$$

where we used (#) and $\widehat{\sigma_\star}(\xi) = 1$ in the last equality. Moreover, for arbitrary $\psi \in C_c(G)$ a direct calculation using (#) and the definition of c_ξ shows

$$\langle E_T(\{\xi\}) f_\psi - \widehat{\psi} c_\xi, E_T(\{\xi\}) f_\psi - \widehat{\psi} c_\xi \rangle = 0.$$

Thus, $E_T(\{\xi\}) f_\psi = \widehat{\psi} c_\xi$ for every $\psi \in C_c(G)$. □

Corollary 2. *Let (Ω, α) be a TMDS with an α-invariant probability measure m and associated autocorrelation function γ. Let $\mathcal{E}$ be the set of eigenvalues of T. Then, the pure point part $\widehat{\gamma}_{pp}$ of $\widehat{\gamma}$ is given as*

$$\widehat{\gamma}_{pp} = \sum_{\xi \in \mathcal{E}} \langle c_\xi, c_\xi \rangle \delta_\xi.$$

In particular, if T has pure point spectrum then $\gamma = \sum_{\xi \in \mathcal{E}} \langle c_\xi, c_\xi \rangle \delta_\xi$.

Proof. The characterizing property of c_ξ given in the previous theorem shows that a ξ with $c_\xi \neq 0$ is an eigenvalue with eigenfunction c_ξ. The formula for the norm of c_ξ in the previous theorem then gives the first statement. Now, the second statement follows by noting that (7) together with pure point spectrum of T implies pure point diffraction (see [62, 40, 3] as well) and, hence, $\widehat{\gamma} = \widehat{\gamma}_{pp}$. □

Let us finish this section by discussing how the considerations from the beginning of this section dealing with point sets and diffraction as a limit fall into the measure framework.

To do so we first note that it is possible to express γ (defined via the closed formula (6)) via a limiting procedure in the ergodic case. The following holds [3].

Theorem 4. *Assume that the locally compact abelian G has a countable base of topology. Let (Ω, α) be a TMDS with ergodic measure m and (B_n) a van Hove sequence along which the Birkhoff ergodic theorem holds. Then, $\frac{1}{|B_n|}\omega_{B_n} * \widetilde{\omega_{B_n}}$ converges to γ_m vaguely for m-almost every $\omega \in \Omega$.*

Next, we show how to consider point sets as measures. The set of discrete point sets in G will be denoted by $\mathcal{D}$. Then,

$$\delta : \mathcal{D} \longrightarrow \mathcal{M}(G), \delta_\Lambda := \sum_{x\in\Lambda} \delta_x,$$

is injective. In this way, $\mathcal{D}$ can and will be identified with a subset of $\mathcal{M}(G)$. In particular, it inherits the vague topology. A subset Λ of G is called *relatively dense* if there exists a compact $C \subset G$ with

$$G = \bigcup_{x\in\Lambda}(x + C)$$

and it is called *uniformly discrete* if there exists an open neighbourhood $U \subset G$ of the origin such that

$$(x + U) \cap (y + U) = \emptyset \tag{8}$$

for all $x, y \in \Lambda$ with $x \neq y$. The set of uniformly discrete sets satisfying (8) is denoted by $\mathcal{D}_U$. An element $\Lambda \in \mathcal{D}_U$ (considered as an element of $\mathcal{M}(G)$) is in fact translation bounded. In particular, we can define the hull of Λ as the closure

$$\Omega(\Lambda) := \overline{\{x + \Lambda : x \in G\}}.$$

Then, $\Omega(\Lambda)$ is a compact TMDS.

6. The Bombieri/Taylor conjecture for general systems

In this section we consider a TMDS (Ω, α) and ask for existence of certain Fourier type coefficients. These coefficients will be given as limits of certain averages. These averages will be defined next.

Definition 3. *Let (Ω, α) be a TMDS. For $\xi \in \widehat{G}$ and $B \subset G$ relatively compact with non-empty interior the function $c_B^\xi : \Omega \longrightarrow C(\Omega)$ is defined by*

$$c_B^\xi(\omega) := \frac{1}{\theta_G(B)} \int_B \overline{(\xi, s)} d\omega(s).$$

The conjecture of Bombieri/Taylor was originally phrased in the framework of point dynamical systems over $\mathbb{Z}$, see [10, 11, 23, 25]. In our context a specific version of it may be reformulated as saying that

$$\widehat{\gamma}(\{\xi\}) = \lim_{n\to\infty} |c_{B_n}^\xi(\omega)|^2,$$

where the limit has to be taken in a suitable sense (see introduction for further discussion).

Our abstract result reads as follows.

Theorem 5. *Let (Ω, α) be a TMDS with an α-invariant probability measure m and associated autocorrelation function γ. Let $\xi \in \widehat{G}$ be arbitrary and $c_\xi \in L^2(\Omega, m)$ be given by Theorem 3. Then, the following assertions hold:*

(a) For every van Hove sequence (B_n) the functions $c_{B_n}^{\xi}$ converge in $L^2(\Omega, m)$ to c_ξ and

$$\widehat{\gamma}(\{\xi\}) = \langle c_\xi, c_\xi \rangle = \lim_{n\to\infty} \langle c_{B_n}^{\xi}, c_{B_n}^{\xi} \rangle.$$

(b) If m is ergodic, the function $|c_\xi|^2$ is almost everywhere equal to $\widehat{\gamma}(\{\xi\})$. Then, $c_{B_n}^{\xi}$ converge almost everywhere to c_ξ, whenever (B_n) is a van Hove sequence along which the Birkhoff ergodic theorem holds. In particular, the functions $|c_{B_n}^{\xi}|^2$ converge almost everywhere to $\widehat{\gamma}(\{\xi\})$.

(c) If (Ω, α) is uniquely ergodic, then the following assertions are equivalent:

(i) *$c_{B_n}^{\xi}$ converges uniformly for one (and then any) van Hove sequence.*

(ii) *c_ξ is a continuous function satisfying $c_\xi(\alpha_{-s}\omega) = (\xi, s)c_\xi(\omega)$ for every $s \in G$ and $\omega \in \Omega$.*

(iii) *$c_\xi \equiv 0$ or ξ is a continuous eigenvalue.*

In these cases $\widehat{\gamma}(\{\xi\}) = \lim_{n\to\infty} |c_{B_n}^{\xi}|^2(\omega)$ uniformly on Ω.

Remark. The parts (a) and (b) of the theorem are new. As discussed in the introduction, validity of variants of (c) is hinted at in the literature, see e.g. [23, 25, 64, 33]. However, so far no proof has been given. For so called model sets and primitive substitutions validity of (i) in (c) has been shown by in [23] and [20] respectively. These proofs do not use continuity of eigenfunctions. On the other hand, continuity of eigenfunctions is known for so-called model sets [62] and primitive substitution systems [65, 66] (see [27] for the one-dimensional situation). Thus, (c) combined with these results on continuity of eigenfunctions gives a new proof for the validity of Bombieri/Taylor conjecture for these systems.

The theorem gives immediately the following corollary, which proves one version of the Bombieri/Taylor conjecture.

Corollary 3. *Let (Ω, α) be a uniquely ergodic TMDS with an α-invariant probability measure m and associated autocorrelation function γ. Then,*

$$\{\xi \in \widehat{G} : \widehat{\gamma}(\{\xi\}) > 0\} = \{\xi \in \widehat{G} : c_{B_n}^{\xi} \text{ does not converge uniformly to } 0\}.$$

Remark. The corollary gives an efficient method to prove $\widehat{\gamma}(\{\xi\}) > 0$, viz it suffices to show that $c_{B_n}^{\xi}(\omega)$ does not converge to zero for a single ω. The corollary is less useful in proving $\widehat{\gamma}(\{\xi\}) = 0$, as in this case one has to check uniform convergence to zero. This shortcoming will be addressed for special systems in the final section of the paper.

Corollary 4. *Let (Ω, α) be a uniquely ergodic TMDS with an α-invariant probability measure m and associated autocorrelation function γ. The following assertions are equivalent:*

(i) *$\widehat{\gamma}$ is a pure point measure and $c_{B_n}^{\xi}$ converges uniformly for every $\xi \in \widehat{G}$.*

(ii) *$L^2(\Omega, m)$ has an orthonormal basis consisting of continuous eigenfunctions.*

Proof. As shown in Theorem 7 of [3], $\widehat{\gamma}$ is a pure point measure if and only if $L^2(\Omega, m)$ has an orthonormal basis consisting of eigenfunctions. We are thus left with the statement on continuity of eigenfunctions.

Here, $(ii) \Longrightarrow (i)$ follows from (c) of the previous theorem. The implication $(i) \Longrightarrow (ii)$ follows from Theorem 8 in [3] applied with $\mathcal{V} := \overline{Lin\{f_\varphi : \varphi \in C_c(G)\}} \subset L^2(\Omega, m)$ after one notices that assumption (i) implies by the previous theorem that all eigenfunctions of the restriction of T to $\mathcal{V}$ are continuous. $\square$

We will give the proof of the theorem at the end of this section. In order to do so, we need some preparatory results.

Lemma 6. *Let $C > 0$ and $V \subset G$ be open, relatively compact and non-empty. Then, for every compact $K \subset G$ and every van Hove sequence (B_n)*

$$\lim_{n\to\infty} \frac{1}{\theta_G(B_n)} \sup\{|\mu|(\partial^K B_n) : \mu \in \mathcal{M}_{C,V}(G)\} = 0.$$

Proof. For a fixed $\mu \in \mathcal{M}_{C,V}(G)$, the corresponding statement is shown by Schlottmann in Lemma 1.1 of [62]. Inspection of the proof shows that convergence to zero holds uniformly on $\mathcal{M}_{C,V}(G)$ (see [37] for a different proof as well). $\square$

Lemma 7. *Let (Ω, α) be a TMDS with $\Omega \subset \mathcal{M}_{C,V}(G)$. Then, for every $\varphi \in C_c(G)$, and $B \subset G$ open relatively compact and non-empty the estimate*

$$\|A_B^\xi(f_\varphi) - \widehat{\varphi}(\xi)c_B^\xi\|_\infty \leq \frac{C_\varphi}{\theta_G(B)} \Big(\sup\{|\mu|(\partial^{S(\varphi)} B) : \mu \in \mathcal{M}_{C,V}(G)\} + \theta_G(\partial^{S(\varphi)} B) \Big)$$

holds, where $S(\varphi) := supp(\varphi) \cup (-supp(\varphi))$ and $C_\varphi := \int |\varphi| dt + \sup\{\int |\varphi|\, d|\mu| : \mu \in \mathcal{M}_{C,V}(G)\}$.

Proof. Define $D(\omega) := \theta_G(B)^{-1} |A_B^\xi(f_\varphi)(\omega) - \widehat{\varphi}(\xi) c_B^\xi(\omega)|$. Then,

$$\begin{aligned} D(\omega) &= \frac{1}{\theta_G(B)} \left| \int_G \int_B \overline{(\xi,t)} \varphi(t-r) dt d\omega(r) - \int_B \int_G \overline{(\xi,t)} \varphi(t-r) dt d\omega(r) \right| \\ &\leq \frac{1}{\theta_G(B)} \left| \int_{G\setminus B} \int_B \overline{(\xi,t)} \varphi(t-r) dt d\omega(r) \right| + \left| \int_B \int_{G\setminus B} \overline{(\xi,t)} \varphi(t-r) dt d\omega(r) \right|. \end{aligned}$$

It is then straightforward to estimate the first term by $\frac{C_\varphi}{\theta_G(B)} |\omega|(\partial^{S(\varphi)} B)$ and the second term by $\frac{C_\varphi}{\theta_G(B)} \theta_G(\partial^{S(\varphi)} B)$. $\square$

The next lemma is the crucial link between Wiener/Wintner type averages and the Fourier coefficient type averages. It shows that the behavior of $A_{B_n}^\xi(f_\varphi)$ is "the same" as the behavior of $\widehat{\varphi}(\xi) c_{B_n}^\xi$ for large $n \in \mathbb{N}$.

Lemma 8. *Let (Ω, α) be a TMDS with Ω and (B_n) an arbitrary van Hove sequence. Let $\xi \in \widehat{G}$ be arbitrary. Then,*

$$\|A_{B_n}^\xi(f_\varphi) - \widehat{\varphi}(\xi) c_{B_n}^\xi\|_\infty \longrightarrow 0,\ n \longrightarrow \infty$$

for every $\varphi \in C_c(G)$.

Proof. This is a direct consequence of Lemma 7 and Lemma 6. $\square$

Proof of Theorem 5. Choose $\sigma \in C_c(G)$ with $\int_G \sigma(s) ds = 1$ and define $\sigma_\star \in C_c(G)$ by $\sigma_\star := (\xi, \cdot)\sigma$. Then, $\widehat{\sigma_\star}(\xi) = 1$ and according to Theorem 3 we have

$$\widehat{\gamma}(\{\xi\}) = \langle c_\xi, c_\xi \rangle$$

with $c_\xi = E_T(\{\xi\}) f_{\sigma_\star}$. This will be used repeatedly below.

(a) From Lemma 1 and definition of c_ξ, we infer

$$\widehat{\gamma}(\{\xi\}) = \langle c_\xi, c_\xi\rangle = \lim_{n\to\infty}\langle A^\xi_{B_n}(f_{\sigma_\star}), A^\xi_{B_n}(f_{\sigma_\star})\rangle.$$

Now, the statement follows from Lemma 8.

(b) As $c_\xi = E_T(\{\xi\})f_{\sigma_\star}$, the function c_ξ is zero or an eigenfunction to ξ. Thus, for fixed $s\in G$, $c_\xi(\alpha_{-s}\omega) = (\xi,s)c_\xi(\omega)$ for almost every $\omega\in\Omega$. In particular, the function $|c_\xi|^2$ is invariant under α and thus, by ergodicity, almost surely equal to a constant. As m is a probability measure this constant is equal to $\langle c_\xi, c_\xi\rangle$, which in turn equals $\widehat{\gamma}(\{\xi\})$.

The statement on almost sure convergence follows from Lemma 8 as $A^\xi_{B_n}(f_{\sigma_\star})$ almost surely converges according to Lemma 2.

(c) This follows from Lemma 8, Theorem 1 and the already shown part. □

As a by-product of our proof we obtain the following result.

Corollary 5. *Let γ be the autocorrelation of a TMDS (Ω,α). Let (B_n) be an arbitrary van Hove sequence. Let $\xi\in\widehat{G}$ be given. Then,*

$$\widehat{\gamma}(\{\xi\}) = \lim_{n\to\infty}\frac{1}{\theta_G(B_n)}\int_{B_n}\overline{(\xi,s)}d\gamma(s)$$

and, similarly,

$$\widehat{\gamma}(\{\xi\}) = \lim_{n\to\infty}\gamma*\varphi_n*\widetilde{\varphi_n}(0)$$

for $\varphi_n := \frac{1}{\theta_G(B_n)}(\xi,\cdot)\,\chi_{B_n}*\sigma$, where σ is an arbitrary element of $C_c(G)$ satisfying $\int_G\sigma dt = 1$.

Remark. Results of this type play an important role in the study of diffraction on $\mathbb{R}^d$ [23, 25, 67]. They do not seem to be known in the generality of locally compact, σ-compact Abelian groups we are dealing with here. They can be inferred, however, from Theorem 11.4 of [21] whenever transformability of $\widehat{\gamma}$ is known. This transformability in turn seems, however, not to be known in general.

Proof. We only consider the first equation. The second statement can be shown with a similar and in fact simpler proof.

Choose $\sigma\in C_c(G)$ and $\varphi_n\in C_c(G)$ as in the statement, i.e. with $\int_G\sigma(s)ds = 1$ and $\varphi_n := \frac{1}{\theta_G(B_n)}(\xi,\cdot)\,\chi_{B_n}*\sigma$. Define $\sigma_\star\in C_c(G)$ by $\sigma_\star := (\xi,\cdot)\sigma$. Then a direct calculation shows

$$\widetilde{\sigma_\star}*\varphi_n(t) = (\xi,t)\frac{1}{\theta_G(B_n)}a_n(t)$$

with

$$a_n(t) = \int_G\int_G\overline{\sigma(s)\sigma(-r)}\chi_{B_n}(t+s-r)drds.$$

Thus, with $K := \operatorname{supp}(\sigma)-\operatorname{supp}(\sigma)$, we have $a_n(t)=0$ for $t\in G\setminus(B_n\cup\partial^K B_n)$, $a_n(t)=1$ for $t\in B_n\setminus\partial^K B$ and $0\le|a_n(t)|\le 1$ for $t\in\partial^K B$. As (B_n) is a van Hove sequence and γ is translation bounded, we then easily infer from Lemma 6 that

$$\widehat{\gamma}(\{\xi\}) = \lim_{n\to\infty}\frac{1}{\theta_G(B_n)}\int_{B_n}\overline{(\xi,s)}d\gamma(s)\quad\text{if and only if}\quad\widehat{\gamma}(\{\xi\}) = \lim_{n\to\infty}\gamma*\widetilde{\sigma_\star}*\varphi_n(0).$$

The latter equality can be shown as follows: A direct calculation shows $A^{\xi}_{B_n}(f_{\sigma_\star}) = f_{\varphi_n}$. Thus, (6), Lemma 1 and Theorem 3 show

$$\gamma * \widetilde{\sigma_\star} * \varphi_n(0) = \langle f_{\sigma_\star}, f_{\varphi_n}\rangle = \langle f_{\sigma_\star}, A^{\xi}_{B_n}(f_{\sigma_\star})\rangle \longrightarrow \langle f_{\sigma_\star}, E_T(\{\xi\}) f_{\sigma_\star}\rangle = \widehat{\gamma}(\{\xi\})$$

and the proof is finished. □

7. Cut and project models and their relatives

In this section we apply the results of the preceding section to model sets and some variants thereof. Model sets were introduced by Meyer in [44] quite before the actual discovery of quasicrystals. A motivation of his work is the quest for sets with a very lattice-like Fourier expansion theory. In fact, model sets can be thought of to provide a very natural generalization of the concept of a lattice. Together with primitive substitutions they have become the most prominent examples of aperiodic order. Accordingly, they have received quite some attention. We refer the reader to [46, 48, 62] for background and further references.

A *cut and project scheme* over G consists of a locally compact abelian group H, called the internal space, and a lattice $\widetilde{L}$ in $G \times H$ such that the canonical projection $\pi : G \times H \longrightarrow G$ is one-to-one between $\tilde{L}$ and $L := \pi(\widetilde{L})$ and the image $\pi_{\text{int}}(\widetilde{L})$ of the canonical projection $\pi_{\text{int}} : G \times H \longrightarrow H$ is dense. Given these properties of the projections π and π_{int}, one can define the $\star$-map $(.)^\star : L \longrightarrow H$ via $x^\star := \big(\pi_{\text{int}} \circ (\pi|_L)^{-1}\big)(x)$, where $(\pi|_L)^{-1}(x) = \pi^{-1}(x) \cap \tilde{L}$, for all $x \in L$.

We summarize the features of a cut- and project scheme in the following diagram:

$$\begin{array}{ccccc}
G & \xleftarrow{\ \pi\ } & G \times H & \xrightarrow{\ \pi_{\text{int}}\ } & H \\
\cup & & \cup & & \cup \text{ dense} \\
L & \xleftarrow{\ 1-1\ } & \tilde{L} & \longrightarrow & L^\star \\
\| & & & & \| \\
L & & \xrightarrow{\qquad\quad \star \qquad\quad} & & L^\star
\end{array}$$

We will assume that the Haar measures on G and on H are chosen in such a way that a fundamental domain of $\tilde{L}$ has measure 1. Given a cut and project scheme, we can associate to any $W \subset H$, called the *window*, the set

$$\curlywedge(W) \;:=\; \{x \in L : x^\star \in W\}$$

A set of the form $t + \curlywedge(W)$ is called *model set* if the window W is relatively compact with nonempty interior. Without loss of generality, we may assume that the stabilizer of the window,

$$H_W \;:=\; \{c \in H : c + W = W\},$$

is the trivial subgroup of H, i.e., $H_W = \{0\}$. A model set is called *regular* if ∂W has Haar measure 0 in H. Any model set turns out to be uniformly discrete.

A central result on model sets (compare [46, 62] and references given there) states that regular model sets are pure point diffractive, i.e. $\widehat{\gamma}$ is a pure point measure. In fact, the associated dynamical system $(\Omega(\Lambda), \alpha)$ obtained by taking the closure $\Omega(\Lambda)$ of $\{t + \Lambda : t \in G\}$ in $\mathcal{M}(G)$ is uniquely ergodic with pure point spectrum with continuous eigenfunctions and the diffraction measure can be calculated explicitely [23, 25, 62]. Given the material of the previous sections we can easily reproduce the corresponding results. This is discussed next. The underlying idea is that the dynamical system "almost agrees" (in the sense of being an almost one-to-one extension) with the so called torus parametrization.

A cut and project scheme gives rise to a dynamical system in the following way: Define $\mathbb{T} := (G \times H)/\widetilde{L}$. By assumption on $\widetilde{L}$, $\mathbb{T}$ is a compact abelian group. Let

$$G \times H \longrightarrow \mathbb{T}, \ \ (t,k) \mapsto [t,k],$$

be the canonical quotient map. Then, there are canonical group homomorphisms

$$\kappa : H \longrightarrow \mathbb{T}, \ \ h \mapsto [0,h], \ \text{ and } \ \iota : G \longrightarrow \mathbb{T}, \ \ t \mapsto [t,0].$$

By the defining properties of a cut and project scheme the homomorphism ι has dense range as $L^\star$ and the homomorphism κ is injective. There is an action α' of G on $\mathbb{T}$ via

$$\alpha' : G \times \mathbb{T} \longrightarrow \mathbb{T}, \ \ \alpha'_t([s,k]) := \iota(-t) + [s,k] = [s-t,k].$$

The dynamical system $(\mathbb{T},\alpha')$ is minimal and uniquely ergodic, as ι has dense range. Moreover, it has pure point spectrum. In fact, the dual group $\widehat{\mathbb{T}}$ gives a set of eigenfunctions, which form a complete orthonormal basis by Peter-Weyl theorem. These eigenfunctions can be described in terms of characters on G and H via the the dual lattice $\widetilde{L}^\perp$ of $\widetilde{L}$ given by

$$\widetilde{L}^\perp := \{(k,u) \in \widehat{G} \times \widehat{H} : k(l)u(l^\star) = 1 \ \ \text{for all } (l,l^\star) \in \widetilde{L}\}.$$

More precisely, standard reasoning gives that $\widehat{\mathbb{T}}$ can naturally be identified with $\widetilde{L}^\perp$. In this identification $(k,u) \in \widetilde{L}^\perp$ corresponds to $\xi \in \widehat{\mathbb{T}}$ with $\xi([t,h]) = k(t)u(h)$. This ξ can then easily be seen to be an eigenfunction to the eigenvalue k.

It turns out that k already determines ξ as will be shown next. Let L° be the set of all $k \in \widehat{G}$ for which there exists $u \in \widehat{H}$ with $(k,u) \in \widetilde{L}^\perp$. As $\pi_2(\widetilde{L})$ is dense in H, we infer that $(k,u),(k,u') \in \widetilde{L}^\perp$ implies $u = u'$. Thus, there exists a unique map $\star : L^\circ \longrightarrow \widehat{H}$ such that

$$\tau : L^\circ \longrightarrow \widetilde{L}^\perp, \ \ k \mapsto (k,k^\star),$$

is bijective.

Having discussed the dynamical behavior of $(\mathbb{T},\alpha')$ we now come to the connection between $\Omega(\Lambda)$ and $\mathbb{T}$. This connection is known under the name of torus parametrization [62, 49]. In Proposition 7 in [5] the following version is given.

Proposition 1. *There exists a continuous G-map $\beta : \Omega(\Lambda) \longrightarrow \mathbb{T}$ such that $\beta(\Gamma) = (t,h) + \widetilde{L}$ if and only if $t + ⅄(W^\circ - h) \subset \Gamma \subset t + ⅄(W - h)$.*

For regular model sets, the Haar measure of the boundary of W is zero. Thus, the previous proposition shows that the set of points in $\mathbb{T}$ with more than one inverse image under β has measure zero. This gives easily (see e.g. [62, 5]) that (Ω,α) inherits unique ergodicity and pure point spectrum with continuous eigenfunctions and eigenvalues $k \in L^\circ$ from $\mathbb{T}$. By Corollary 2 the diffraction measure can then be written as

$$\widehat{\gamma} = \sum_{k \in L^\circ} \langle c_k, c_k \rangle \delta_k.$$

It remains to determine the c_k. By continuity of the eigenfunctions and Theorem 5, the c_k arise as the uniform limit of the function $c^k_{B_n}$, where (B_n) is an arbitrary van Hove sequence. For $k \in L^\circ$ the calculation of this limit can be performed using a convergence result for cut and project schemes known as uniform distribution. Using the uniform distribution result of [47] one obtains

$$c_k(\Gamma) = \overline{\tau(k)(\beta(\Gamma))} \int_W (k^\star, y) dy$$

for $k \in L^\circ$. Putting the previous two equations together we obtain

$$\widehat{\gamma} = \sum_{k \in L^\circ} A_k \delta_k \text{ with } A_k = \left| \int_W (k^\star, y) dy \right|^2.$$

We refrain from giving further details here but refer to the next subsection, where a more general situation is treated.

7.1. **Deformed model sets.** In this subsection we discuss a special form of perturbation of model sets leading to deformed model sets. These sets have attracted attention in recent years [4, 9, 22]. Based on the results of the previous sections and [4], it is possible to calculate diffraction measure and eigenfunctions. Details are worked out in [38]. Here, we only sketch the results.

We keep the notation used so far. Let $\Lambda := \curlywedge(W)$ be a model set with a regular window. Let Ω be its hull. By the discussion above, Ω is uniquely ergodic with invariant probability measure m. Let now a continuous function $\vartheta : W \longrightarrow G$ be given. This map gives rise to to the perturbed measure

$$\omega_\vartheta := \sum_{x \in \Lambda} \delta_{x + \vartheta(x^*)}.$$

Denote its hull (in $\mathcal{M}(G)$) by Ω_ϑ. As shown in [4] there exists a unique G-invariant continuous map

$$\Phi_\vartheta : \Omega \longrightarrow \Omega_\vartheta$$

with $\Phi_\vartheta(\Lambda) = \omega_\vartheta$ and Ω_ϑ inherits unique ergodicity with pure point spectrum and continuous eigenfunctions c_k^ϑ to the eigenvalues $k \in L^\circ$ from Ω. Thus, again by Corollary 2, $\widehat{\gamma}^\vartheta$ is a pure point measure which can be written as $\widehat{\gamma}^\vartheta = \sum_{k \in L^\circ} \langle c_k^\vartheta, c_k^\vartheta \rangle \delta_k$. By Theorem 5, each c_k^ϑ a limit of $c_{B_n}^k$. Using uniform distribution [47], we infer that the limit exists and equals

$$c^k(\Gamma) = \overline{\tau(k)(\beta(\Gamma))} \int_W (k^\star, y) \overline{(k, \vartheta(y))} dy$$

for $k \in L^\circ$. We also obtain that the limits are identically zero for $k \notin L^\circ$. Accordingly, we find

$$\widehat{\gamma}^\vartheta = \sum_{k \in L^\circ} A_k \delta_k, \text{ with } A_k := \left| \int_W (k^\star, y) \overline{(k, \vartheta(y))} dy \right|^2.$$

Note that with $\vartheta \equiv 0$ we regain the case of regular model sets.

7.2. **Cut and project models based on measures.** In this subsection we shortly discuss the measure variant of model sets studied in [37] (see [56] as well). Based on the results of the previous sections, it is possible to calculate diffraction and eigenfunctions in this case. This is carried out in [37]. Here, we only sketch the main ideas.

Definition 4. (a) *A quadruple* $(G, H, \widetilde{L}, \rho)$ *is called a* measure cut and project scheme *if* $(G, H, \widetilde{L})$ *is a cut and project scheme and* ρ *is an* $\widetilde{L}$*-invariant Borel measure on* $G \times H$.
(b) *Let* $(G, H, \widetilde{L}, \rho)$ *be a measure cut and project scheme. A function* $f : H \longrightarrow \mathbb{C}$ *is called* admissible *if it is measurable, locally bounded and for arbitrary* $\varepsilon > 0$ *and* $\varphi \in C_c(G)$ *there exists a compact* $Q \subset H$ *with*

$$\int_{G \times H} |\varphi(t+s) f(h+k)| (1 - 1_Q(h+k)) \, \mathrm{d}|\rho|(t,h) \le \varepsilon$$

for every $(s,k) \in G \times H$, *where* 1_Q *denotes the characteristic function of* Q.

An example of a measure cut and project scheme is given by a cut and project scheme $(G, H, \widetilde{L})$ and $\rho := \delta_{\widetilde{L}} := \sum_{x \in \widetilde{L}} \delta_x$. It is not hard to see that then every Riemann integrable $f : H \longrightarrow \mathbb{C}$ is admissible. In this way regular model sets fall within this framework.

Given a measure cut and project scheme $(G, H, \widetilde{L}, \rho)$ with an admissible f the map

$$\nu_f : C_c(G) \longrightarrow \mathbb{C}, \;\; \varphi \mapsto \int_{G \times H} \varphi(t) f(h) \, \mathrm{d}\rho(t,h),$$

is a translation bounded measure. Thus, we can consider its hull

$$\Omega(\nu_f) := \overline{\{\alpha_t(\nu_f) : t \in G\}}.$$

This hull is a TMDS.

Assume for the remainder of this section that f is not only admissible but also continuous. Then, it turns out that $(\Omega(\nu_f), \alpha)$ is minimal, uniquely ergodic and has pure point spectrum with continuous eigenfunctions with set of eigenvalues contained L°. In fact, the map

$$\mu : \mathbb{T} \longrightarrow \Omega(\nu_f), \;\; \mu([s,k])(\varphi) = \int f(h+k) \varphi(s+t) \, \mathrm{d}\rho(t,h)$$

is a continuous surjective G-map and $(\Omega(\nu_f), \alpha)$ inherits pure point spectrum with continuous eigenfunctions from $(\mathbb{T}, \alpha)$. Note that in terms of factor maps the situation here is somehow opposite to the situation considered in the last subsection: The dynamical system in question $(\Omega(\nu_f), \alpha)$ is a factor of the torus and not the other way round!

By pure point spectrum with eigenvalues contained in L° we can write $\widehat{\gamma} = \sum_{k \in L^{\circ}} \langle c_k, c_k \rangle \delta_k$ by Corollary 2. Again, by Theorem 5, the c_k can be calculated as a uniform limit. The calculation of the limit requires some care. The outcome is

$$c_k(\mu([s,h])) = \tau(k)([s,h]) \frac{\rho_{\mathbb{T}}(\lambda)}{(m_G \times m_H)_{\mathbb{T}}(1)} \int f(u) \, (k^{\star}, y) \; \mathrm{d}y.$$

Here, $\rho_{\mathbb{T}}$ is the unique measure on $\mathbb{T}$ with

$$\int_{G \times H} g(s,h) \, \mathrm{d}\rho(s,h) = \int_{\mathbb{T}} \sigma_{\xi}(g) \, \mathrm{d}\rho_{\mathbb{T}}(\xi)$$

for all $g \in C_c(G \times H)$, where $\sigma_{\xi}(g) = \sum_{(l,l^{\star}) \in \widetilde{L}} g(s+l, h+l^{\star})$ for $g \in C_c(G \times H)$. Thus, we end up with

$$\widehat{\gamma} = \sum_{k \in L^{\circ}} A_k \delta_k, \;\; \text{with} \;\; A_k = |\frac{\rho_{\mathbb{T}}(\tau(k))}{(m_G \times m_H)_{\mathbb{T}}(1)} \int_H f(u)(k^{\star}, y) \; \mathrm{d}y|^2.$$

Note that (at least formally) we regain the formula for regular model sets by choosing $\rho = \delta_{\widetilde{L}}$ and f to be a characteristic function.

Remark. As shown in [37], the set $\Omega(\nu_f)$ carries a natural structure of a compact abelian group and μ is a continuous group homomorphism.

8. Examples with randomness

In this section we study diffraction for randomizations of systems with aperiodic order. We will be particularly interested in models arising via percolation process and models arising via a random displacement (sometimes also known as Mott type disorder). Both percolation and random displacement models can be thought of to give a more realistic description of the

solid in question: Percolation takes into account that defects arise. Random displacement takes into account the thermal movement of the atoms in the solid. Our results will show that in these cases validity of a (variant) of the Bombieri/Taylor conjecture is still true! Note that both models rely on perturbations via independent identically distributed random variables.

As discussed in the introduction, Percolation and Random displacement models based on aperiodic order have been investigated earlier [26, 50, 24, 30, 31]. Here, we would like to emphasize the work of Külske [30, 31]. This work gives strong convergence statements for approximants of the diffraction measure for rather general situations containing both percolation and random displacement models. In fact, [31] can even treat situations with non i.i.d. random variables. Restricted to our setting this provides convergence for expressions of the form

$$\frac{1}{|B_n|}\int I_{\Lambda\cap B_n}(k)\varphi(k)dk$$

for an arbitrary but fixed φ from the space of Schwartz functions. As this requires the smoothing with φ, it does not seem to give any Bombieri/Taylor type of convergence statement. In this sense, our results below provide a natural complement to his corresponding results of [30].

Our construction of the percolation model and the proof of its ergodicity seem to be new. In fact, we present a unified approach to construction and proof of ergodicity for percolation models and random displacement models. This may be of independent interest.

We will be interested in point sets and measures in Euclidean space. Thus, our group is given as $G=\mathbb{R}^d$. The σ-algebra generated by the vague topology is called Borel σ-algebra It can be described as follows. A cylinder set is a finite union of sets of the form

$$\{\mu\in\mathcal{M}(G) : f_{\varphi_j}(\mu)\in I_j, j=1,\ldots,n\}$$

with $n\in\mathbb{N}$, $\varphi_j\in C_c(G)$, and $I_j\subset\mathbb{C}$ measurable. Here, f_φ is defined in (5). The support of such a cylinder set is given as the union of the supports of all functions φ involved. In particular, the support of a cylinder set is always compact.

Lemma 9. *Let $\Omega\subset\mathcal{M}(G)$ be compact. Then, the set of cylinder sets in Ω is an algebra (i.e. closed under taking complements and finite intersections) and generates the Borel-σ-algebra.*

Proof. The set of cylinder sets is obviously closed under taking finite intersections and complements. It generates the Borel-σ-algebra by its very definition. □

Lemma 10. *Let $\Omega\subset\mathcal{M}(G)$ be a compact α-invariant set and m an ergodic measure on (Ω,α). Let (ν^ω) be a family of probability measures on $\mathcal{M}(G)$ satisfying the following properties:*

1. *$\omega\mapsto\nu^\omega(f)$ is measurable for any nonnegative measurable f on $\mathcal{M}(G)$.*
2. *$\nu^{\alpha_t\omega}(f)=\nu^\omega(f(\alpha_t\cdot))$ for all $t\in G$ and $\omega\in\Omega$.*
3. *There exists a constant $D>0$ with $\nu^\omega(B\cap C)=\nu^\omega(B)\nu^\omega(C)$ whenever B and C are cylinder sets with supports of distance bigger than D.*

Then, the measure $m^{(\nu)}$ on $\mathcal{M}(G)$ with

$$m^{(\nu)}(f)=\int_\Omega\left(\int f(\mu)d\nu^\omega(\mu)\right)dm(\omega)$$

is ergodic.

Proof. The proof is a variant of the well-known argument showing ergodicity (and, in fact, strong mixing of the Bernoulli shift). Let A be a measurable α invariant set in $\mathcal{M}(G)$. Define $f : \Omega \longrightarrow [0, \infty)$ by $f(\omega) := \nu^\omega(A)$. By the assumptions (1) and (2) on ν and the invariance of A the function f is invariant and measurable. Hence, by ergodicity of m, $\nu^\omega(A) = m^{(\nu)}(A)$ for m almost every $\omega \in \Omega$.

By Lemma 9 the algebra of cylinder sets generates the Borel-σ-algebra. Thus, for any $\varepsilon > 0$, there exists a cylinder set B with $m^{(\nu)}(A \triangle B) \leq \varepsilon$. Here, $\triangle$ denotes the symmetric difference. Let $t \in G$ be arbitrary. Then, triangle inequality for symmetric differences and invariance of A give

$$m^{(\nu)}(B \triangle \alpha_t B) \leq m^{(\nu)}(B \triangle A) + m^{(\nu)}(A \triangle \alpha_t B) \leq 2\varepsilon.$$

As the cylinder set B has compact support we can choose $t \in G$ so that the supports of B and $\alpha_t B$ have distance at least D. Hence, (3) yields

$$\nu^\omega(B \cap \alpha_t B) = \nu^\omega(B)\nu^\omega(\alpha_t B)$$

for all $\omega \in \Omega$. Combining these formulas we obtain

$$2\varepsilon \geq |m(B) - m(B \cap \alpha_t B)| = \int_\Omega \nu^\omega(B)(1 - \nu^\omega(\alpha_t B))dm(\omega).$$

As $m^{(\nu)}(A \triangle B) \leq \varepsilon$, we infer

$$\int_\Omega \nu^\omega(A)(1 - \nu^\omega(\alpha_t B))dm(\omega) \leq 3\varepsilon.$$

As $\nu^\omega(A) = m^{(\nu)}(A)$ almost surely and m is α-invariant this gives

$$m^{(\nu)}(A) - m^{(\nu)}(A)m^{(\nu)}(B) \leq 3\varepsilon.$$

As this can be inferred for any $\varepsilon > 0$ we obtain

$$m^{(\nu)}(A) - m^{(\nu)}(A)^2 = 0.$$

This shows $m^{(\nu)}(A) = 1$ or $m^{(\nu)}(A) = 0$. □

Remark. The proof shows that assumption (3) is stronger than needed. It suffices, to find to each cylinder set with support B a t with $\nu^\omega(B \cap \alpha_t B) = \nu^\omega(B)\nu^\omega(\alpha_t B)$. This type of condition could be required on arbitrary locally compact abelian groups, which are not compact. In fact, even an averaged version of this condition can be seen to be sufficient.

Lemma 11. *Let (c_n) be a bounded sequence of complex numbers and (X_n) a sequence of bounded identically distributed independent random variables with expectation value $E \in \mathbb{C}$. Then,*

$$\frac{1}{n}\sum_{j=1}^{n}(c_j X_j - c_j E) \longrightarrow 0, n \to \infty,$$

almost surely.

Proof. Without loss of generality we can assume that both (c_n) and (X_n) are real-valued. Now, the statement follows from the boundedness assumption on (c_n) and (X_n) by Kolmogorov criterion. □

We will now fix an open relatively compact neighborhood of the origin of $\mathbb{R}^d$ and consider the set $\mathcal{D}_U$ of all uniformly discrete sets with "distance" U between different points. We will say that (Ω, α, m) with $\Omega \subset \mathcal{D}_U$ is a dynamical system if Ω is a compact α-invariant subset of $\mathcal{D}_U$ and m is an α-invariant probability measure on Ω.

8.1. **Percolation models.** In this section we discuss diffraction for percolation models.

Fix $p \in (0,1)$ and let ν_p be the probability measure on $\{0,1\}$ with $\nu_p(\{1\}) = p$. To $\Lambda \in \mathcal{D}_U$ we associate the product space

$$S_\Lambda^P := \prod_{x \in \Lambda} \{0,1\}$$

with product measure $\nu'_\Lambda = \prod_{x\in\Lambda} \nu_p$. The map

$$j_\Lambda^P : S_\Lambda^P \longrightarrow \mathcal{M}(G),\ j_\Lambda(s) := \sum_{x\in\Lambda} s(x)\delta_x$$

allows one to push ν'_Λ to a measure ν^Λ on $\mathcal{M}(G)$ viz we define

$$\nu^\Lambda(f) := \nu'_\Lambda(f \circ j_\Lambda^P).$$

The percolation associated to a dynamical system (Ω, α) with $\Omega \subset \mathcal{D}_U$ is then given by the measure $m^P = m^{(\nu)}$ with

$$m^P(f) = \int_\Omega \left(\int f(\mu) d\nu^\Lambda(\mu) \right) dm(\Lambda).$$

The following theorem has been proven in [26] and extended in [50]. It also follows from Lemma 10 above.

Theorem 6. *The measure m^P is ergodic with support contained in $\mathcal{D}_U$.*

Proof. It suffices to show that assumptions (1), (2) and (3) of Lemma 10 are satisfied. Validity of (2) is clear. (3) follows as ν'_Λ is a product measure. To show (1) it suffices to show that

$$\Lambda \mapsto \nu^\Lambda(f_{\varphi_1} \ldots f_{\varphi_n})$$

is continuous (and hence measurable) for any $n \in \mathbb{N}$ and $\varphi_1, \ldots, \varphi_n \in C_c(G)$. Choose an open relatively compact set U with $U = -U$ containing the supports of all φ_j, $j = 1, \ldots, n$. For $s \in \{0,1\}^{\Lambda\cap U}$ let $\sharp_1 s$ and $\sharp_0 s$ denote the number of 1's and 0's in s respectively. Then, a short calculation gives

$$\nu^\Lambda(f_{\varphi_1} \ldots f_{\varphi_n}) = \sum_{s\in\{0,1\}^{\Lambda\cap U}} \left(\sum_{x\in\Lambda\cap U} s(x)\varphi_1(-x) \right) \cdots \left(\sum_{x\in\Lambda\cap U} s(x)\varphi_n(-x) \right) p^{\sharp_1 s}(1-p)^{\sharp_0(s)}.$$

This easily shows the desired continuity. $\square$

We now turn to diffraction. The autocorrelation of $\gamma^P = \gamma_{m^P}$ can easily be calculated and seen to be $\gamma^P = p^2\gamma_m + p(1-p)\delta_0$. In particular,

$$\widehat{\gamma}^P = p^2 \widehat{\gamma}_m + p(1-p)\,1 \tag{9}$$

contains an absolutely continuous component.

Lemma 12. *Let $\Lambda \in \mathcal{D}_U$ and $\xi \in \widehat{G}$ be given. Let (B_n) be a van Hove sequence in G. If $c_{B_n}^\xi(\Lambda)$ converge to a complex number A, then $c_{B_n}^\xi(\omega)$ converges to pA for ν^Λ almost every $\omega \in \mathcal{D}_U$.*

Proof. It suffices to consider ω of the form $\omega = j_\Lambda(s)$ with $s \in S_\Lambda^P$. The lemma then claims that

$$c_{B_n}^{\xi}(\omega) = \frac{1}{|B_n|}\sum_{x\in\Lambda\cap B_n} s(x)(\xi,x) \longrightarrow p\lim_{n\to\infty}\frac{1}{|B_n|}\sum_{x\in\Lambda\cap B_n}(\xi,x), n\to\infty.$$

By uniform discreteness of Λ, the sequence $\frac{\sharp B_n\cap\Lambda}{|B_n|}$ is bounded. Thus, it suffices to show that

$$\frac{1}{\sharp B_n\cap\Lambda}\sum_{x\in\Lambda\cap B_n}(s(x)-p)(\xi,x)) \longrightarrow 0, n\to\infty.$$

This in turn follows easily from Lemma 11. □

Putting these results together we obtain the following variant of Bombieri/Taylor conjecture.

Theorem 7. *Let (Ω,α,m) with $\Omega\subset\mathcal{D}_U$ be a uniquely ergodic dynamical system with continuous eigenfunctions. Then, for any $\xi\in\widehat{G}$, and $\Lambda\in\Omega$ the averages $c_{B_n}^{\xi}(\omega)$ converge for ν^Λ almost every $\omega\in\mathcal{D}_U$ to a limit $c^\xi(\Lambda)$. This limit depends only on Λ (and not on ω) and satisfies $|c^\xi(\Lambda)|^2 = p^2\widehat{\gamma}_m(\{\xi\}) = \widehat{\gamma}^P(\{\xi\})$. In particular, $|c_{B_n}^{\xi}(\omega)|^2$ converge for m^P almost every $\omega\in\Omega$ to $\widehat{\gamma}^P(\{\xi\})$.*

Proof. As (Ω,α) is uniquely ergodic with continuous eigenfunctions, Theorem 5 gives convergence of $c_{B_n}^{\xi}(\Lambda)$ to continuous functions $c_\xi(\Lambda)$ with $\widehat{\gamma}_m(\{\xi\})\equiv|c_\xi(\Lambda)|^2$ for all $\Lambda\in\Omega$ and $\xi\in\widehat{G}$. The previous lemma then proves the ν^Λ almost sure convergence of $c_{B_n}^{\xi}(\omega)$ for each Λ. This lemma and the explicit formula (9) then show the last statement. □

8.2. **Random displacement models.** In this subsection we consider a random displacement in $G=\mathbb{R}^d$. Fix a probability measure σ on $\mathbb{R}^d$ with bounded range. To $\Lambda\in\mathcal{D}_U$ we associate the space

$$S_\Lambda^{RD} = \prod_{x\in\Lambda}\mathbb{R}^d$$

with product measure $\sigma'_\Lambda = \prod_{x\in\Lambda}\sigma$. The map

$$j_\Lambda^{RD} : S_\Lambda^{RD} \longrightarrow \mathcal{M}(G),\ j_\Lambda^{RD}(s) := \sum_{x\in\Lambda}\delta_{x+s(x)}$$

allows one to push σ'_Λ to a measure σ^Λ on $\mathcal{M}(G)$ viz we define

$$\sigma^\Lambda(f) := \sigma'_\Lambda(f\circ j_\Lambda^{RD}).$$

The random displacement model associated to a dynamical system (Ω,α,m) with $\Omega\subset\mathcal{D}_U$, is then given by the measure $m^{RD} = m^{(\sigma)}$ with

$$m^{RD}(f) = \int_\Omega\left(\int f(\mu)d\sigma^\Lambda(\mu)\right)dm(\Lambda).$$

As Ω is compact and σ is bounded, the support of m^{RD} is compact. The following is a consequence of Lemma 10 above. It seems to be new. The proof is very similar to the proof of Theorem 6. We omit the details.

Theorem 8. *The measure m^{RD} is ergodic.*

We now turn to diffraction. By ergodicity and Theorem 4, the autocorrelation $\gamma^{RD} = \gamma_{m^{RD}}$ can be calculated as a limit almost surely. This limit has been calculated in [24] for a fixed Λ and shown to be

$$\gamma^{RD} = \gamma_m * \sigma * \widetilde{\sigma} + n_0(\delta_0 - \sigma * \widetilde{\sigma}),$$

where n_0 is the density of points. In particular,

$$\widehat{\gamma}^{RD} = |\widehat{\sigma}|^2 \widehat{\gamma}_m + n_0(1 - |\widehat{\sigma}|^2) \tag{10}$$

contains an absolutely continuous component.

The next lemma and the following theorem can now be proven along very similar lines as the corresponding results in the previous subsection. We omit the details.

Lemma 13. *Let $\Lambda \in \mathcal{D}_U$ and $\xi \in \widehat{G}$ be given. Let (B_n) be a van Hove sequence in G. If $c^{\xi}_{B_n}(\Lambda)$ converge to a complex number A, then $c^{\xi}_{B_n}(\omega)$ converges to $\widehat{\sigma}(\xi)A$ for σ^{Λ} almost every $\omega \in \mathcal{M}(G)$.*

Proof.

Theorem 9. *Let (Ω, α, m) with $\Omega \subset \mathcal{D}_U$ be a uniquely ergodic dynamical system with continuous eigenfunctions. Then, for any $\xi \in \widehat{G}$, and $\Lambda \in \Omega$ the averages $c^{\xi}_{B_n}(\omega)$ converge for σ^{Λ} almost every $\omega \in \mathcal{M}(G)$ to a limit $c^{\xi}(\Lambda)$. This limit depends only on Λ (and not on ω) and satisfies $|c^{\xi}(\Lambda)|^2 = \widehat{\gamma}_m(\{\xi\})|\widehat{\sigma}(\xi)|^2 = \widehat{\gamma}^{RD}(\{\xi\})$. In particular, $|c^{\xi}_{B_n}(\omega)|^2$ converge for m^{RD} almost every $\omega \in \Omega$ to $\widehat{\gamma}^{RD}(\{\xi\})$.*

$\square$

Remark. The above considerations rely essentially on the independent identical distribution of the randomness and the locallity of the randomness. Therefore, various further models can be treated by the same line of reasoning. In particular, we could treat models combining random displacement with percolation.

9. Linearly repetitive systems

In this section we discuss linearly repetitive Delone dynamical systems and their subshift counterparts known as linearly recurrent subshifts. We will refer to both classes as LR-systems. Such systems were introduced recently in [16, 34] and have further been studied e.g. in [13, 12, 15]. In fact, LR-systems are brought as models for perfectly ordered quasicrystals [34]. Thus, validity of the Bombieri/Taylor conjecture for these systems is a rather relevant issue.

LR-systems can be thought of as generalized primitive substitution systems [16]. As continuity of eigenfunctions is known for primitive substitutions [65, 66], it is natural to assume that continuity holds for LR-systems as well. Somewhat surprisingly, this turns out to be wrong as discussed in [12]. Thus, validity of the Bombieri/Taylor conjecture can not be derived from the material presented so far for these models.

It is nevertheless true as shown below. More generally, we show that for these systems the modules $|A^{\xi}_{B_n}(f)|$ converge uniformly (while the averages themselves may not converge). The key to these results are the uniform subadditive ergodic theorems from [15, 35]. Let us caution the reader that these results do not hold for arbitrary van Hove sequences (B_n) but rather only for Fisher sequences.

We focus on linearly repetitive Delone dynamical systems in this section and only shortly sketch the subshift case.

A subset of $\mathbb{R}^d$ is called *Delone set* if it is uniformly discrete and relatively dense (see end of Section 5 for definition of these notions). As usual we will identify a uniformly discrete subset of $\mathbb{R}^d$ with the associated translation bounded measure and this will allow us to speak about e.g. the hull $\Omega(\Lambda)$ of a Delone set.

Definition 5. *The open ball with radius R around the origin is denoted by $U_R(0)$. A Delone set Λ is called linearly repetitive if there exists a $C > 0$ such that for all $R \geq 1$, $x \in \mathbb{R}^d$ and $y \in \Lambda$, there exists a $z \in U_{RC}(x) \cap \Lambda$ with*

$$(-z + \Lambda) \cap U_R(0) = (-y + \Lambda) \cap U_R(0).$$

Roughly speaking, linear repetitivity means that a local configuration of of size R can be found in any ball of size CR. If Λ is linearly repetitive, then $\Omega(\Lambda)$ is minimal and uniquely ergodic.

Linearly repetitive systems allow for a uniform subadditive ergodic theorem and this will be crucial to our considerations. The necessary details are given next. A subset of $\mathbb{R}^d$ of the form

$$I_1 \times \ldots \times I_d,$$

with nonempty bounded intervals I_j, $j = 1, \ldots, d$, of $\mathbb{R}$ is called a box. The lengths of the intervals I_j, $j = 1, \ldots, d$, are called the side lengths of the box. The set of boxes with all side lengths between r and $2r$ is denoted by $\mathcal{B}(r)$. The set of all boxes in $\mathbb{R}^d$ will be denoted by $\mathcal{B}$. Lebesgue measure is denoted by $|\cdot|$.

Then Corollary 4.3 of Damanik/Lenz [15] can be phrased as follows (see [35] for related results as well).

Lemma 14. *Let Λ be linearly repetitive. Let $F : \mathcal{B} \longrightarrow \mathbb{R}$ satisfy the following:*

- (P0) *There exists a $C > 0$ such that $|F(B)| \leq C|B|$ for all boxes with minimal side length at least 1.*
- (P1) *There exists a function $b : \mathcal{B} \longrightarrow [0, \infty)$ with $\lim_{n\to\infty} \frac{b(Q_n)}{|Q_n|} = 0$ for any sequence of boxes (Q_n) with minimal side length going to infinity such that*

$$F(\cup_{j=1}^n B_j) \leq \sum_{j=1}^n (F(B_j) + b(B_j)),$$

  whenever $\cup_{j=1}^n B_j$ is a box and the B_j, $j = 1, \ldots, n$, are boxes disjoint up to their boundary.
- (P2) *There exists a function $e : [1, \infty) \longrightarrow [0, \infty)$ with $\lim_{r\to\infty} e(r) = 0$ such that $|F(B) - F(x + B)| \leq e(r)|B|$, whenever $x + B \cap \Lambda = (x + B) \cap \Lambda$ and the minimal side length of B is at least 1.*

Then, for any sequence of boxes (Q_n) with $Q_n \in \mathcal{B}(r_n)$ and $r_n \to \infty$, the limit $\lim_{n\to\infty} \frac{F(Q_n)}{|Q_n|}$ exists and does not depend on this sequence.

Remark. These conditions have simple interpretations. (P1) means that the function F is sub additive up to a boundary term b and (P2) means that F has an asymptotic Λ-invariance property.

Let now Λ be linearly repetitive. As $\Omega(\Lambda)$ is uniquely ergodic, the autocorrelation $\gamma = \gamma_\Gamma$ exists for any $\Gamma \in \Omega(\Lambda)$. Define the set of local patches $P(\Gamma)$ of a Delone set Γ by $P(\Gamma) := \{(-x + \Gamma) \cap U_R(0) : R \geq 0, x \in \Gamma\}$. Minimality implies

$$\Omega(\Lambda) = \{\Gamma : P(\Gamma) = P(\Lambda)\}. \tag{11}$$

In the context of $\mathbb{R}^d$, we can identify $\xi \in \mathbb{R}^d$ with the character $\exp(i\xi\cdot)$ in $\widehat{\mathbb{R}^d}$. For $B \subset \mathbb{R}^d$ relatively compact with non-empty interior, Λ Delone, and $\xi \in \mathbb{R}^d$, we define accordingly

$$C_B^\xi(\Lambda) := c_B^\xi(\delta_\Lambda) = \frac{1}{|B|} \sum_{x \in B \cap \Lambda} \exp(-i\xi x).$$

Now, our result reads as follows.

Theorem 10. *Let Λ be linearly repetitive and γ the associated autocorrelation. Then,*

$$\widehat{\gamma}(\{\xi\}) = \lim_{n\to\infty} |C_{Q_n}^\xi(\Lambda)|^2$$

for any sequence of boxes (Q_n) with $Q_n \in \mathcal{B}(r_n)$ and $r_n \to \infty$.

Proof. Define $F : \mathcal{B} \longrightarrow \mathbb{R}$ by $F(Q) = |\sum_{x\in Q\cap\Lambda} \exp(-i\xi x)|$. Then, F clearly satisfies the conditions $(P0)$, $(P1)$ and $(P2)$ of Lemma 14. Therefore, by Lemma 14, the limit $\lim_{n\to\infty} \frac{F(Q_n)}{|Q_n|}$ exists for any sequence of cubes (Q_n) with $Q_n \in \mathcal{B}(r_n)$ and $r_n \to \infty$ and the limit does not depend on this sequence. By (11), this means that the limit

$$a(\xi) := \lim_{n\to\infty} |C_B^\xi(\Gamma)|$$

exists uniformly in $\Gamma \in \Omega(\Lambda)$ and does not depend on Γ. Now, Theorem 5 (a) gives the desired result. $\square$

We next come to a generalization for arbitrary eigenfunctions.

Proposition 2. *Let Λ be a Delone set and $f : \Omega(\Lambda) \longrightarrow \mathbb{C}$ continuous. Then, there exists a function $e : [1,\infty) \longrightarrow [0,\infty)$ with $\lim_{r\to\infty} e(r) = 0$ and*

$$\int_B |f(\alpha_{-s}\Gamma) - f(\alpha_{-s}\Gamma')| ds \le e(r)|B|$$

whenever B is a box with minimal side length at least r and $\Gamma, \Gamma' \in \Omega(\Lambda)$ with $\Gamma \cap B = \Gamma' \cap B$.

Proof. Define $e(r)$ to be the supremum of the set of terms

$$\frac{1}{|B|} \int_B |f(\alpha_{-s}\Gamma) - f\alpha_{-s}\Gamma')| ds,$$

where B runs over all boxes with minimal side length at least r and Γ, Γ' belong to $\Omega(\Lambda)$ and satisfy $\Gamma \cap B = \Gamma' \cap B$.

Choose $\varepsilon > 0$ arbitrary. As f is continuous, there exists $R > 0$ such that

$$|f(\Gamma) - f(\Gamma')| \le \varepsilon \tag{12}$$

whenever $\Gamma \cap C_R = \Gamma' \cap C_R$, where C_R denotes the cube centered at the origin with side length $2R$. For a box $B = [a_1, b_1] \times \ldots [a_d, b_d]$ with minimal side length bigger than $2R$ set $B_R := [a_1 - R, b_1 - R] \times \ldots [a_d - R, b_d - R]$. Define B_R accordingly if the intervals making up B are not closed. Choose r_0 such that

$$2\frac{|B \setminus B_R|}{|B|} \|f\|_\infty \le \varepsilon \tag{13}$$

for any box B with minimal side length at least r_0. Then, for such a box B and $\Gamma, \Gamma' \in \Omega(\Lambda)$ with $\Gamma \cap B = \Gamma' \cap B$ we have

$$|f(\alpha_{-s}\Gamma) - f(\alpha_{-s}\Gamma')| \leq \varepsilon \tag{14}$$

for all $s \in B_R$ by (12). By (13), we then easily infer $e(r) \leq 2\varepsilon$ whenever $r \geq r_0$. As $\varepsilon > 0$ is arbitrary, this proves the proposition. □

Theorem 11. *Let Λ be linearly repetitive. Let $f : \Omega(\Lambda) \longrightarrow \mathbb{C}$ be continuous. Then, for any sequence of boxes (Q_n) with $Q_n \in \mathcal{B}(r_n)$ and $r_n \to \infty$, the sequence $|A^{\xi}_{Q_n}(f)|$ converges uniformly to $\sqrt{\langle E_T(\{\xi\})f, E_T(\{\xi\})f\rangle}$.*

Proof. Choose $\Gamma \in \Omega(\Lambda)$ arbitrary. Define $F : \mathcal{B} \longrightarrow \mathbb{R}$ by $F(Q) = |\int_Q \exp(-i\xi s) f(\alpha_{-s}(\Gamma)ds|$. Clearly, F satisfies $(P0)$ and $(P1)$ of Lemma 14. Moreover, by the previous proposition it also satisfies $(P2)$. Thus, the limit $\lim_{n\to\infty} |Q_n|^{-1} F(Q_n)$ exists. Another application of the previous proposition and (11) shows that the limit does not depend on the choice of Γ and is uniform in Γ. Now, the claim follows from Lemma 1. □

We finish this section with a short discussion of linearly repetitive subshifts.

Let $\mathcal{A}$ be a finite set called the alphabet and equipped with the discrete topology. Let Ω be a subshift over $\mathcal{A}$. Thus, Ω is a closed subset of $\mathcal{A}^{\mathbb{Z}}$, where $\mathcal{A}^{\mathbb{Z}}$ is given the product topology and Ω is invariant under the shift operator $\alpha : \mathcal{A}^{\mathbb{Z}} \longrightarrow \mathcal{A}^{\mathbb{Z}}$, $(\alpha a)(n) \equiv a(n+1)$.

We consider sequences over $\mathcal{A}$ as words and use standard concepts from the theory of words ([16, 43]). In particular, $\mathrm{Sub}(w)$ denotes the set of subwords of w and the length $|w|$ of the word $w = w(1)\dots w(n)$ is given by n. To Ω we associate the set $\mathcal{W} = \mathcal{W}(\Omega)$ of finite words associated to Ω given by $\mathcal{W} \equiv \cup_{\omega\in\Omega}\mathrm{Sub}(\omega)$. A subshift is called linearly repetitive if there exists a $D > 0$ s.t. every $v \in \mathcal{W}$ is a factor of every $w \in \mathcal{W}$ with $|w| \geq D|v|$.

A function $F : \mathcal{W} \longrightarrow \mathbb{R}$ is called subadditive if it satisfies $F(ab) \leq F(a) + F(b)$. If a subshift is linearly repetitive, the limit $\lim_{|x|\to\infty} \frac{F(x)}{|x|}$ exists for every subadditive F (see [15, 35]). This can be used to obtain the following analogue of the previous theorem.

Theorem 12. *Let (Ω, α) be a linearly repetitive subshift. Let f be a continuous function of Ω and $z \in \mathbb{C}$ with $|z| = 1$ be arbitrary. For $n \in \mathbb{N}$ define the function $A_n(f)$ by $A_n(f)(\omega) := \sum_{k=0}^{n-1} z^{-k} f(\alpha_{-k}\omega)$. Then, $|A_n(f)|$ converge uniformly to the constant function $\sqrt{\langle E_T(\{z\})f, E_T(\{z\})f\rangle}$.*

Proof. Recall that a function f on Ω is called locally constant (with constant $L \in \mathbb{N}$) if $f(\omega) = f(\rho)$ whenever $\omega(-L)\dots\omega(L) = \rho(-L)\dots\rho(L)$. It suffices to show the theorem for locally constant functions, as they are dense in the continuous functions. To a locally constant function f with constant L we associate the function $F : \mathcal{W} \longrightarrow \mathbb{R}$ defined by

$$F(w) \equiv \begin{cases} |w|\|f\|_\infty & : \quad |w| \leq 2L \\ 2L\|f\|_\infty + |\sum_{k=L}^{|w|-L} z^{-k} f(\alpha_k\omega)| & : \quad \text{for } \omega \in \Omega \text{ with } \omega(1)\dots\omega(|w|) = w \text{ if } |w| > 2L. \end{cases}$$

As f is locally constant this is well defined. It is not hard to see that F is subadditive. As discussed above, then the limit $\lim_{|x|\to\infty} \frac{F(x)}{|x|}$ exists. This easily yields the statements. □

Let us finish this section by emphasizing the following subtle point: As continuity of eigenfunctions fails for general LR-systems, we can not appeal to the results of the previous section to obtain validity of $(**)$ for LR-systems. This does not exclude, however, the possibility that all eigenfunctions relevant to Bragg peaks are continuous. We consider this an interesting question.

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